



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:50 AM UTC

PDB ID : 7LHD / pdb_00007lhd
EMDB ID : EMD-23336
Title : The complete model of phage Qbeta virion
Authors : Chang, J.Y.; Zhang, J.
Deposited on : 2021-01-22
Resolution : 4.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

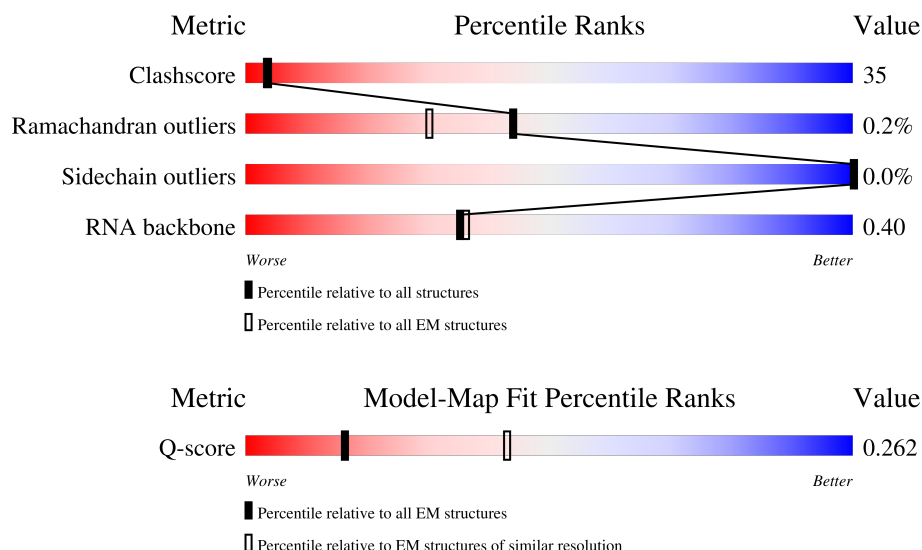
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2407 (4.10 - 5.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4217	57% 30% 52% 17%
2	M	420	48% 64% 35%
3	B	133	92% 74% 25%

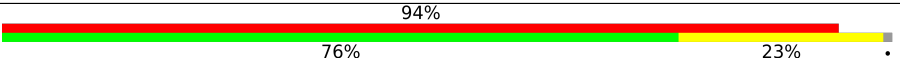
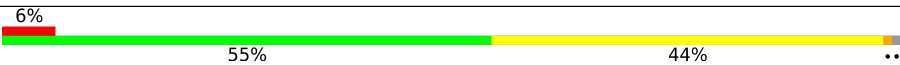
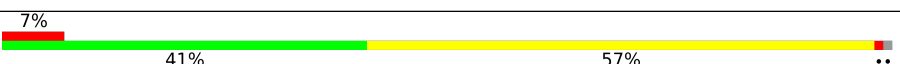
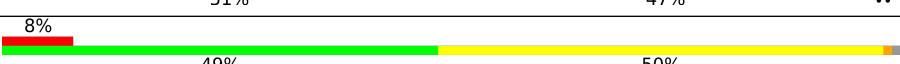
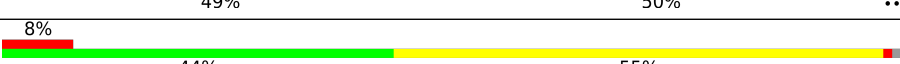
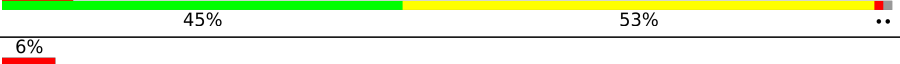
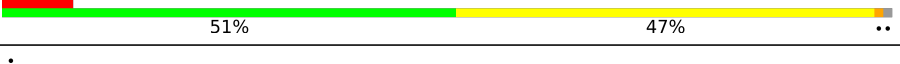
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Mol	Chain	Length	Quality of chain
3	BA	133	
3	BB	133	
3	BC	133	
3	BD	133	
3	BE	133	
3	BF	133	
3	BG	133	
3	BH	133	
3	BI	133	
3	BJ	133	
3	BK	133	
3	BL	133	
3	BM	133	
3	BN	133	
3	CA	133	
3	CB	133	
3	CC	133	
3	CD	133	
3	CE	133	
3	CF	133	
3	CG	133	
3	CH	133	
3	CI	133	
3	CJ	133	
3	CK	133	

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Mol	Chain	Length	Quality of chain
3	CL	133	
3	CM	133	
3	CN	133	
3	D	133	
3	DA	133	
3	DB	133	
3	DC	133	
3	DD	133	
3	DE	133	
3	DF	133	
3	DG	133	
3	DH	133	
3	DI	133	
3	DJ	133	
3	DK	133	
3	DL	133	
3	DM	133	
3	DN	133	
3	EA	133	
3	EB	133	
3	EC	133	
3	ED	133	
3	EE	133	
3	EF	133	
3	EG	133	

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Mol	Chain	Length	Quality of chain
3	EH	133	
3	EI	133	
3	EJ	133	
3	EK	133	
3	EL	133	
3	EM	133	
3	EN	133	
3	FA	133	
3	FB	133	
3	FC	133	
3	FD	133	
3	FE	133	
3	FF	133	
3	FG	133	
3	FH	133	
3	FI	133	
3	FJ	133	
3	FK	133	
3	FL	133	
3	FM	133	
3	FN	133	
3	GA	133	
3	GB	133	
3	GC	133	
3	GD	133	

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Mol	Chain	Length	Quality of chain
3	GE	133	
3	GF	133	
3	GG	133	
3	GH	133	
3	GI	133	
3	GJ	133	
3	GK	133	
3	GL	133	
3	GM	133	
3	GN	133	
3	HA	133	
3	HB	133	
3	HC	133	
3	HD	133	
3	HE	133	
3	HF	133	
3	HG	133	
3	HH	133	
3	HI	133	
3	HJ	133	
3	HK	133	
3	HL	133	
3	HM	133	
3	HN	133	
3	IA	133	

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Mol	Chain	Length	Quality of chain
3	IB	133	
3	IC	133	
3	ID	133	
3	IE	133	
3	IF	133	
3	IG	133	
3	IH	133	
3	II	133	
3	IJ	133	
3	IK	133	
3	IL	133	
3	IM	133	
3	IN	133	
3	JA	133	
3	JB	133	
3	JC	133	
3	JD	133	
3	JE	133	
3	JF	133	
3	JG	133	
3	JH	133	
3	JI	133	
3	JJ	133	
3	JK	133	
3	JL	133	

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Mol	Chain	Length	Quality of chain
3	JM	133	
3	JN	133	
3	KA	133	
3	KB	133	
3	KC	133	
3	KD	133	
3	KE	133	
3	KF	133	
3	KG	133	
3	KH	133	
3	KI	133	
3	KJ	133	
3	KK	133	
3	KL	133	
3	KM	133	
3	KN	133	
3	LA	133	
3	LB	133	
3	LC	133	
3	LD	133	
3	LE	133	
3	LF	133	
3	LG	133	
3	LH	133	
3	LI	133	

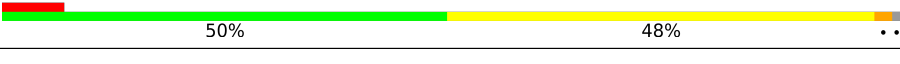
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Mol	Chain	Length	Quality of chain
3	LJ	133	
3	LK	133	
3	LL	133	
3	LM	133	
3	LN	133	
3	MA	133	
3	MB	133	
3	MC	133	
3	MD	133	
3	ME	133	
3	MF	133	
3	MG	133	
3	MH	133	
3	MI	133	
3	MJ	133	
3	MK	133	
3	ML	133	
3	MM	133	
3	MN	133	
3	NA	133	
3	NB	133	
3	NC	133	
3	ND	133	
3	NE	133	
3	NF	133	

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Mol	Chain	Length	Quality of chain
3	NG	133	 8% 51% 47% ..
3	NH	133	 6% 50% 48% ..
3	NI	133	 5% 51% 47% ..
3	NJ	133	 7% 50% 48% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 271383 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Genomic RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4217	Total	C	N	O	P	0	0
			89319	39933	15385	29784	4217		

- Molecule 2 is a protein called Maturation protein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	419	Total	C	N	O	S	0	0
			3438	2210	615	610	3		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	D	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BA	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BB	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BC	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BD	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BE	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BF	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BG	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BH	132	Total	C	N	O	S	0	0
			993	616	177	198	2		
3	BI	132	Total	C	N	O	S	0	0
			993	616	177	198	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	BK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	BL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	BM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	BN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	CN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DB	132	Total 993	C 616	N 177	O 198	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	DC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	DN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	ED	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EI	132	Total 993	C 616	N 177	O 198	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	EJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	EN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FD	122	Total 930	C 582	N 166	O 182		0	0
3	FE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	FN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GB	124	Total 942	C 588	N 168	O 185	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	GC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	GN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HI	132	Total 993	C 616	N 177	O 198	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	HJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	HN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	ID	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	II	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	IN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JB	132	Total 993	C 616	N 177	O 198	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	JC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	JN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KI	132	Total 993	C 616	N 177	O 198	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	KJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	KN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LL	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	LN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MB	132	Total 993	C 616	N 177	O 198	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	MC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MD	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	ME	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MG	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MH	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MI	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MJ	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MK	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	ML	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MM	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	MN	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	NA	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	NB	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	NC	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	ND	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	NE	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	NF	132	Total 993	C 616	N 177	O 198	S 2	0	0
3	NG	132	Total 993	C 616	N 177	O 198	S 2	0	0
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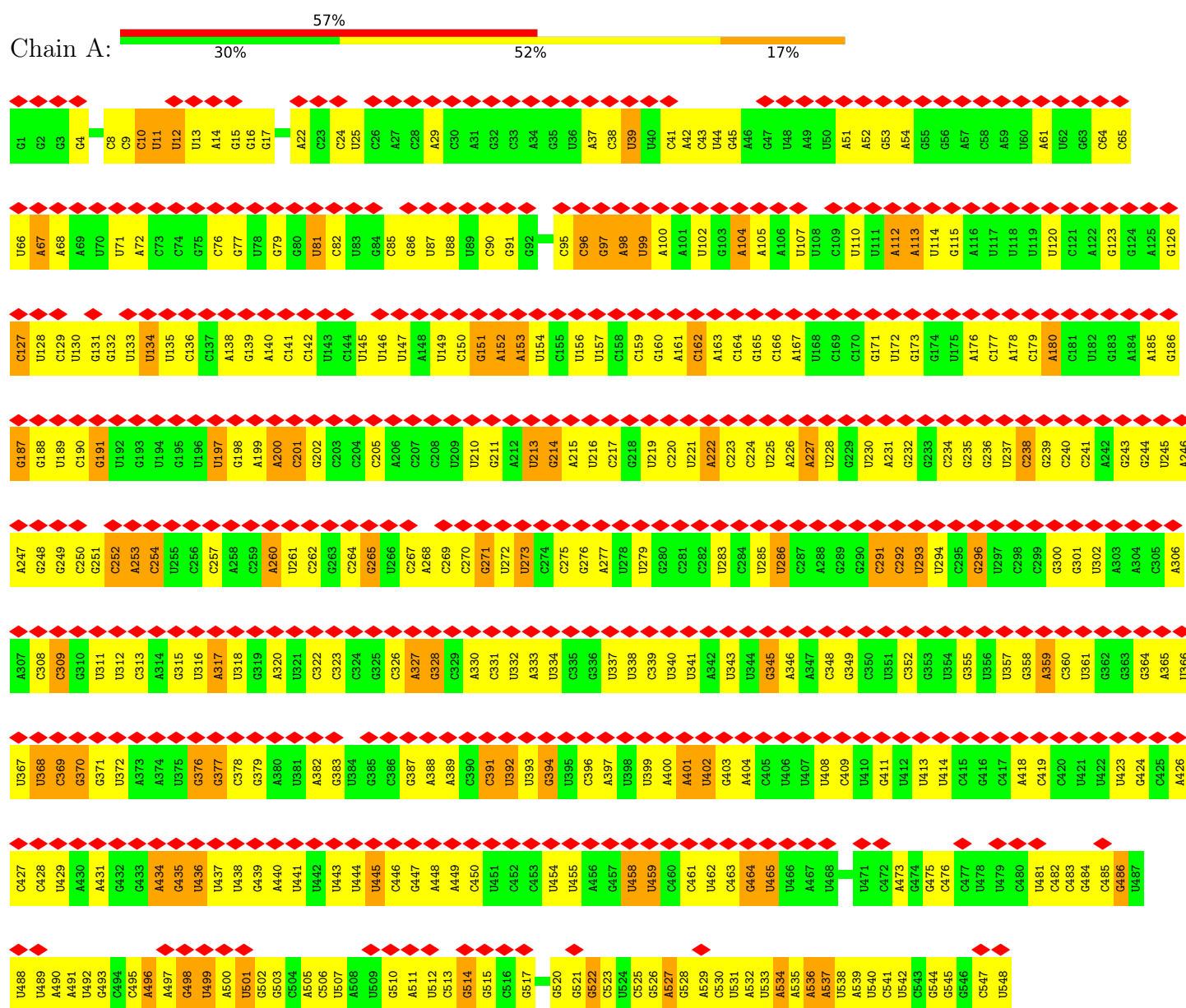
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	NJ	132	Total	C	N	O	S	0	0
			993	616	177	198	2		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

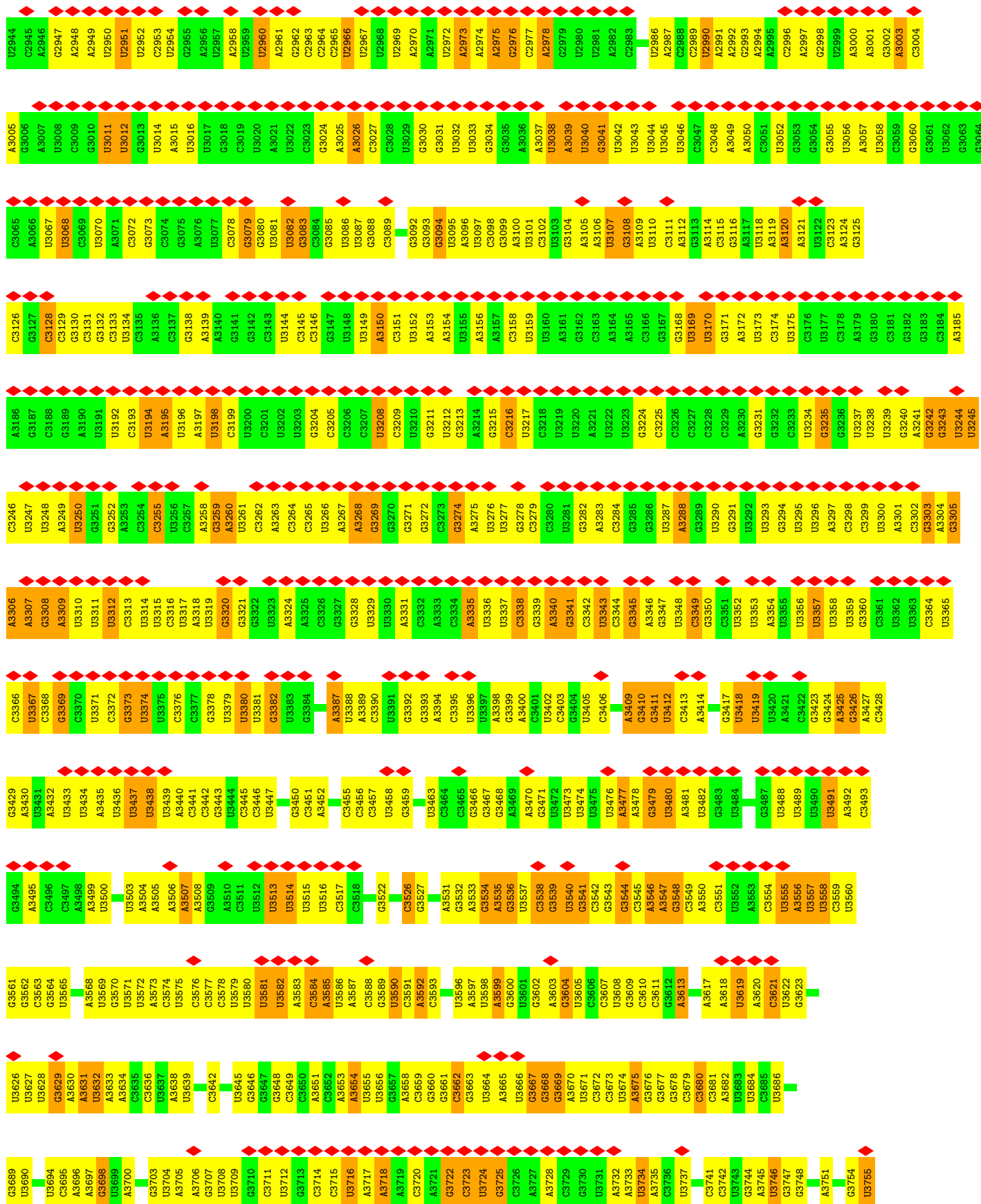
• Molecule 1: Genomic RNA

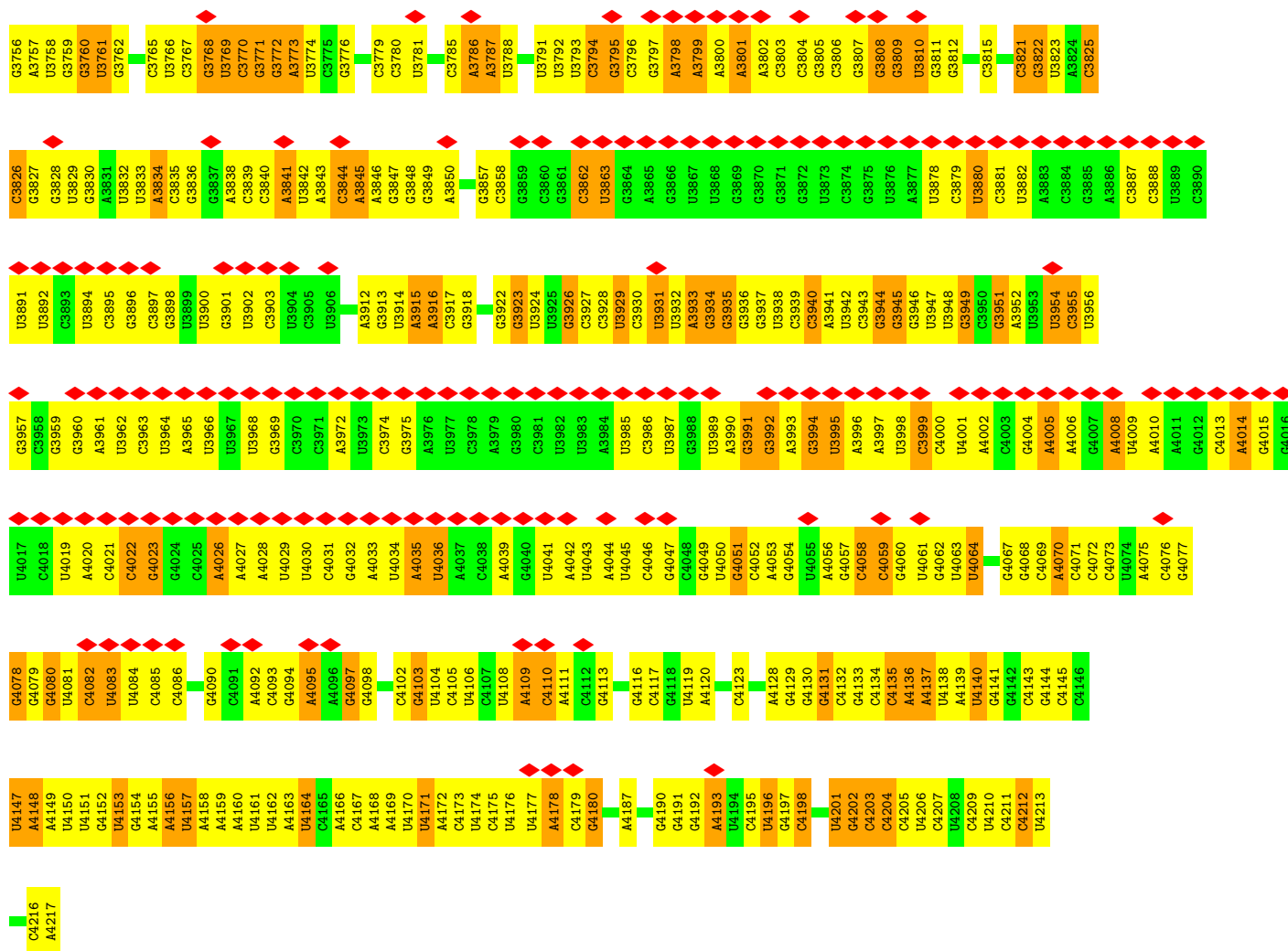


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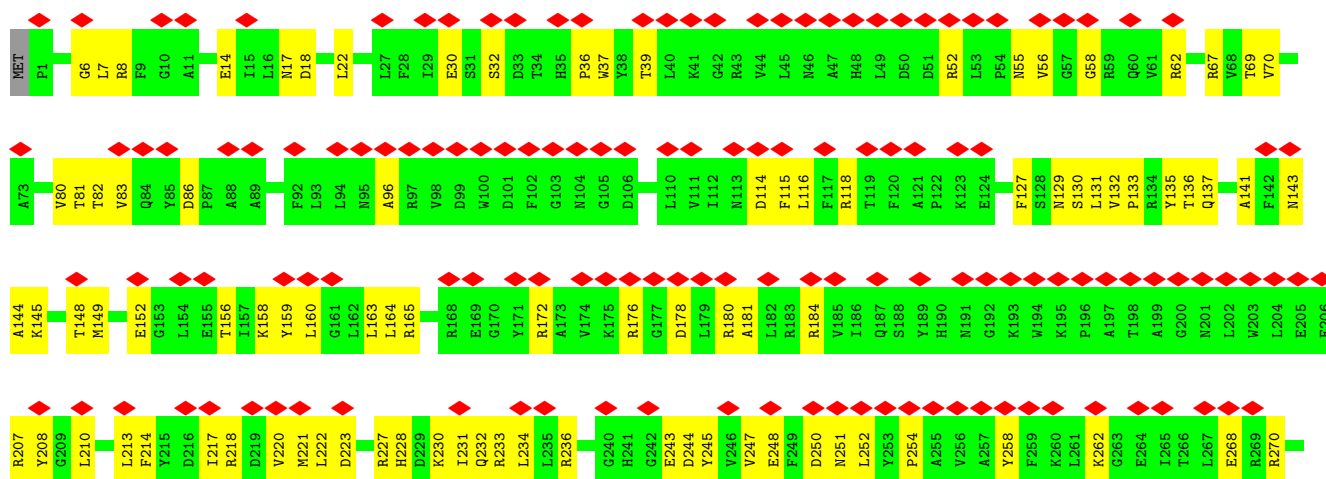
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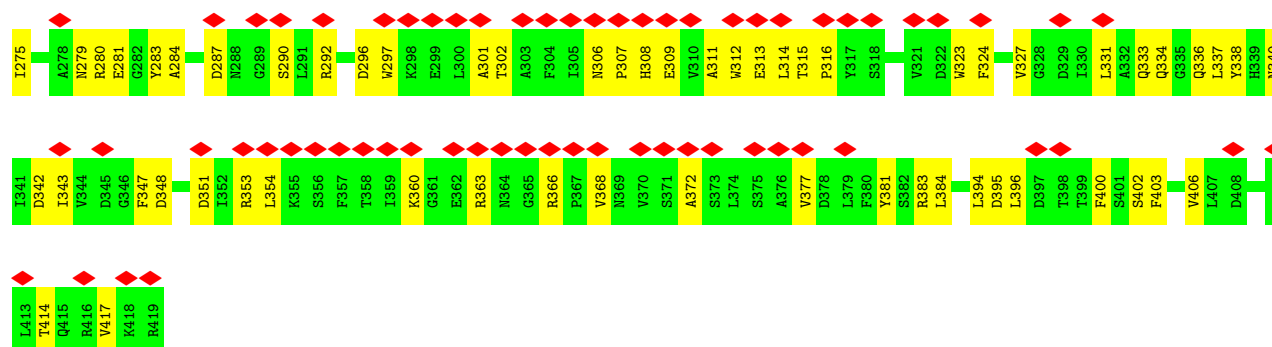
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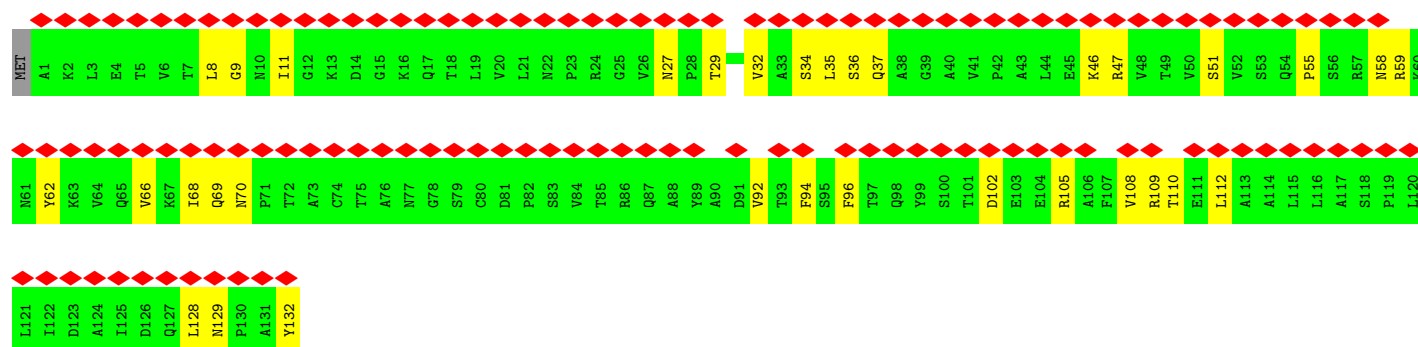
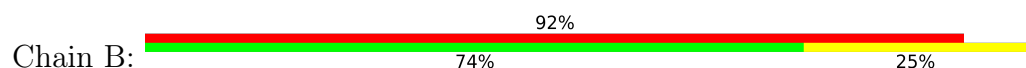


• Molecule 2: Maturation protein A2

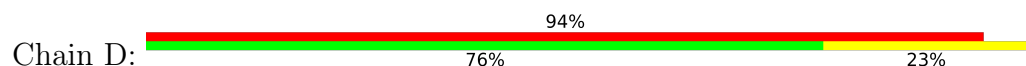




• Molecule 3: Capsid protein



• Molecule 3: Capsid protein

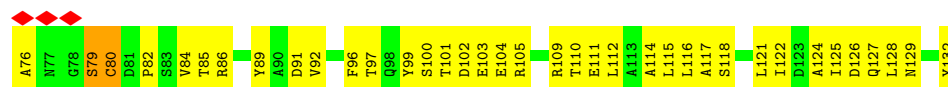
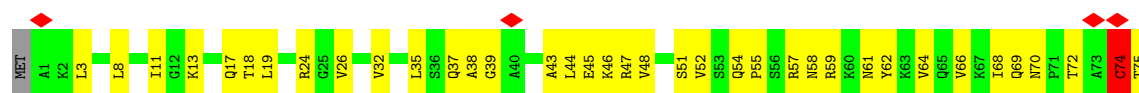
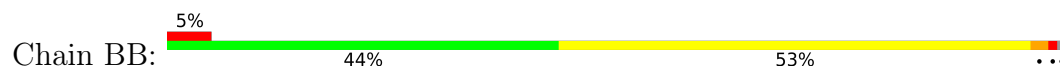


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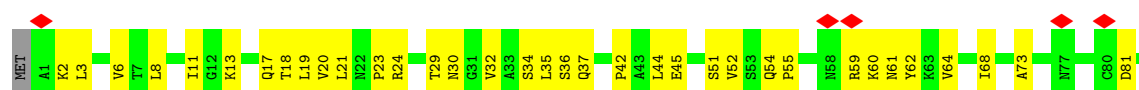




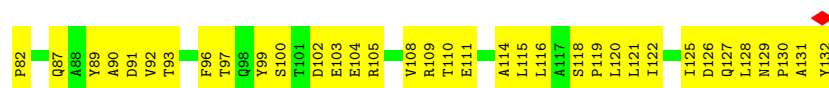
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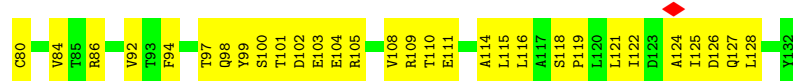
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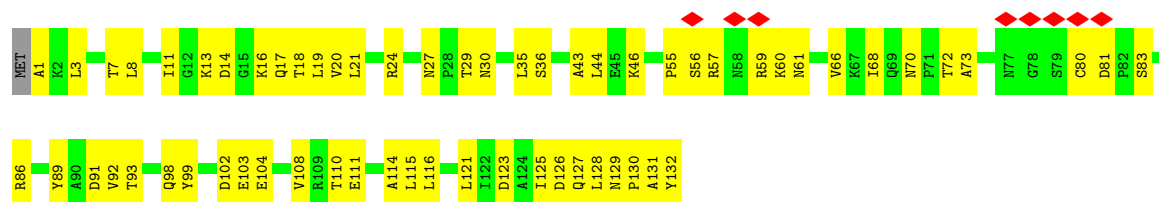
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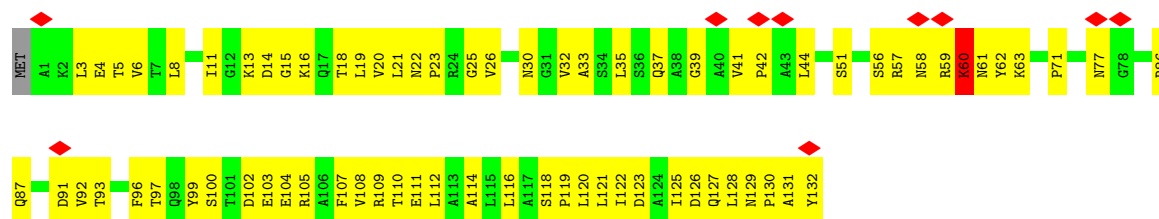
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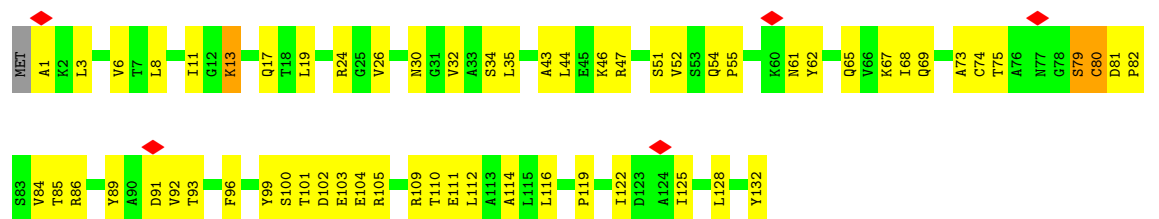
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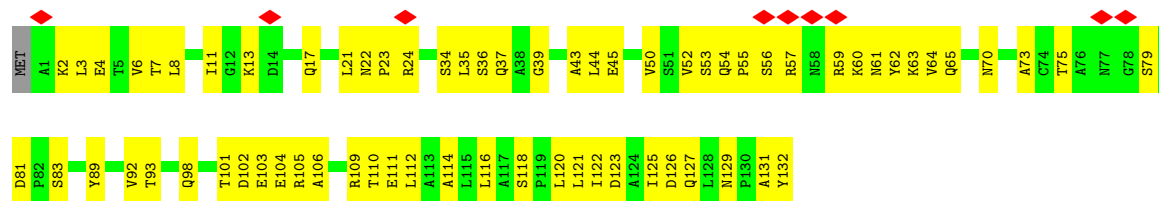
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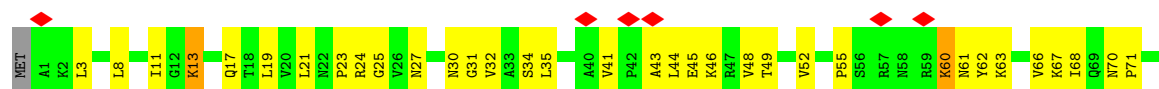
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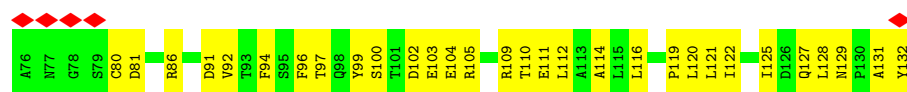


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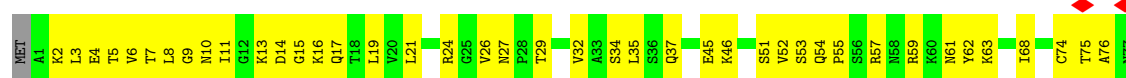


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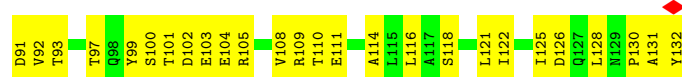
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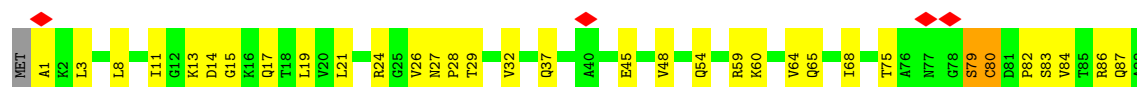
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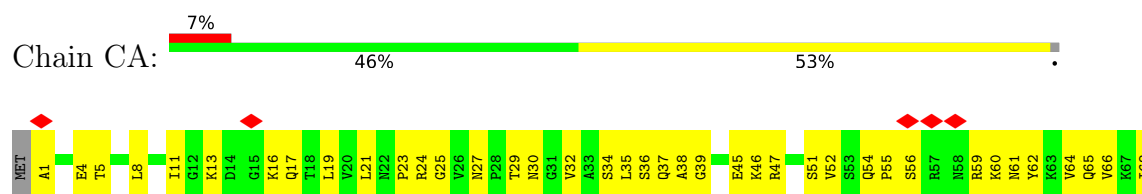
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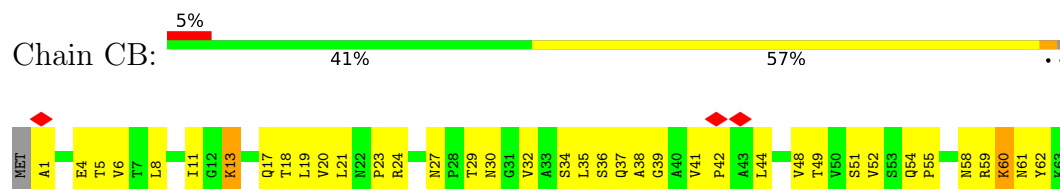
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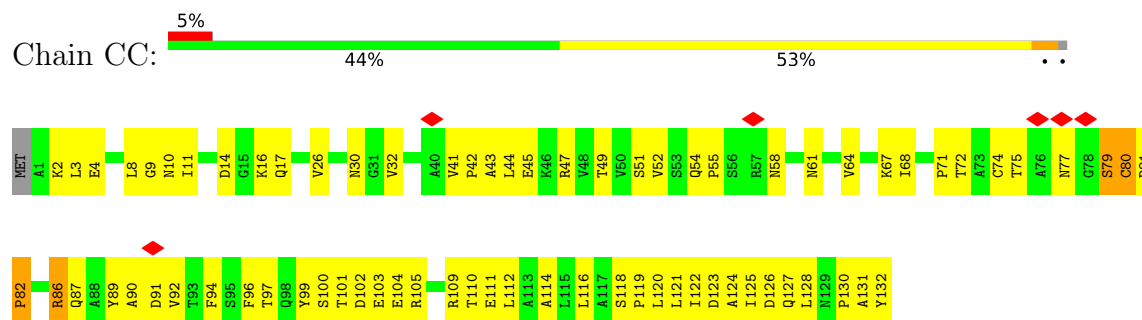
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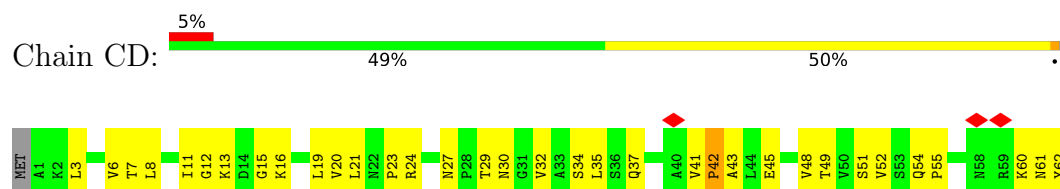
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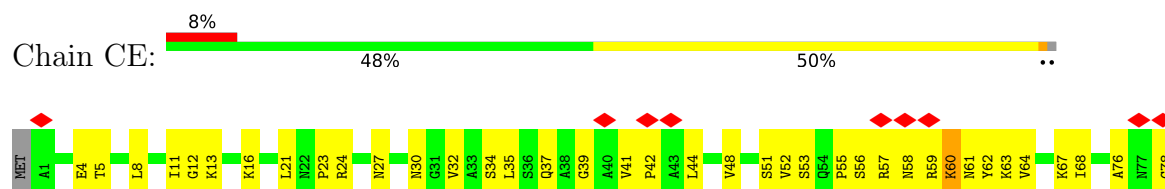
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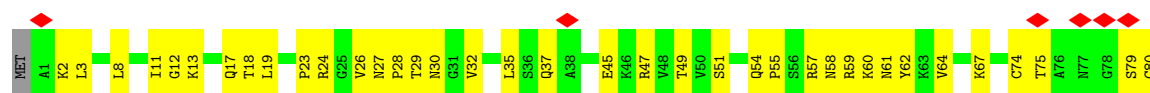


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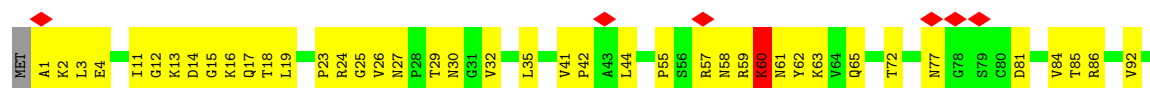
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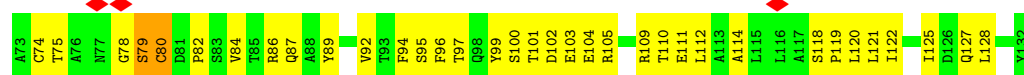
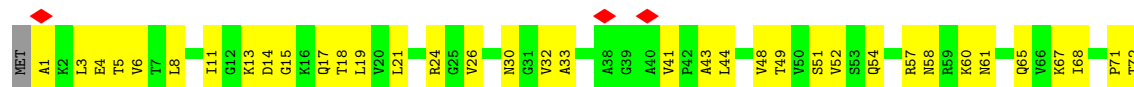
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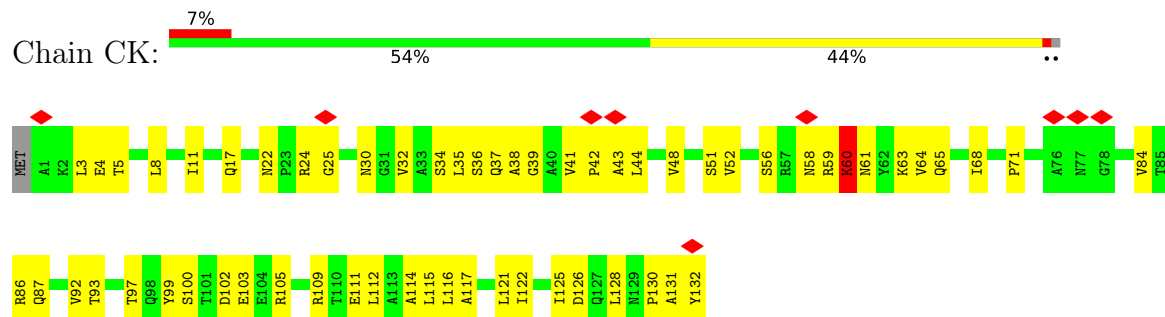
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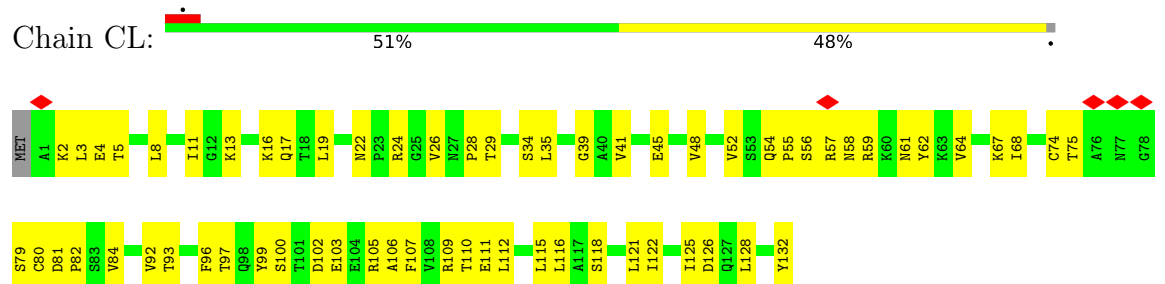
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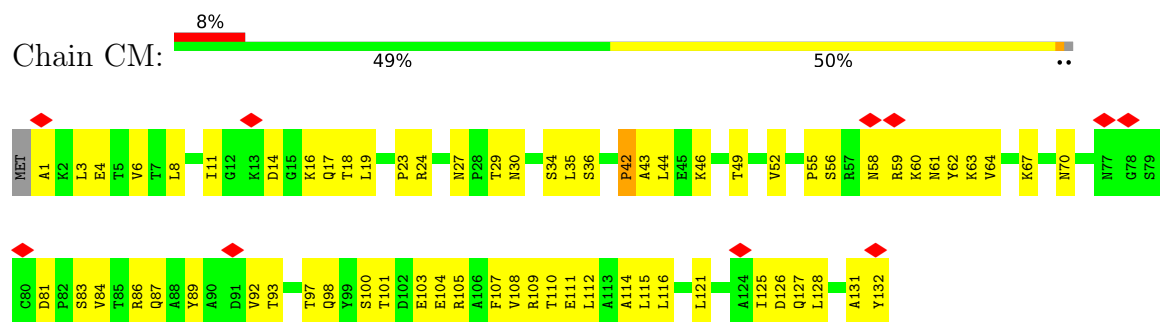
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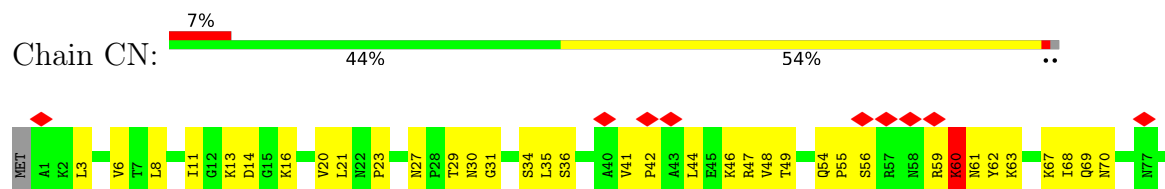
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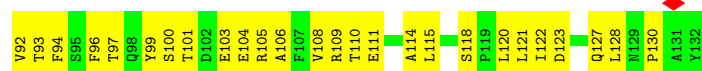
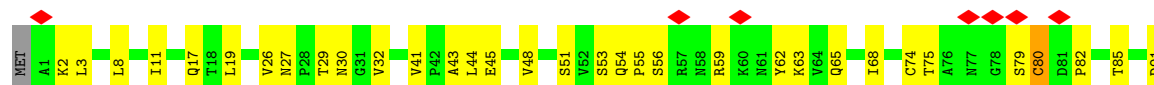


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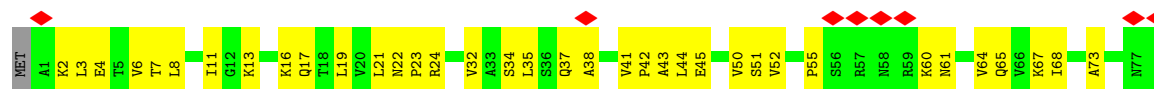




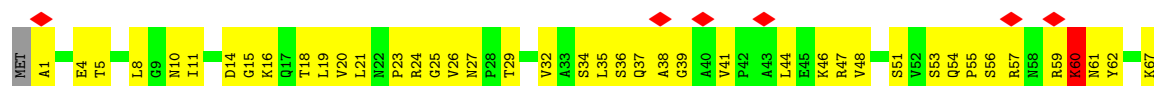
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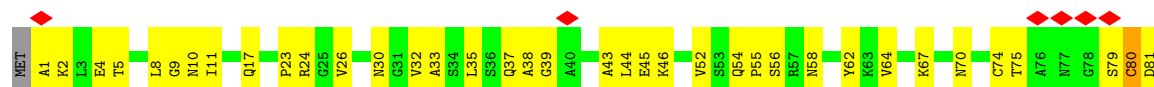
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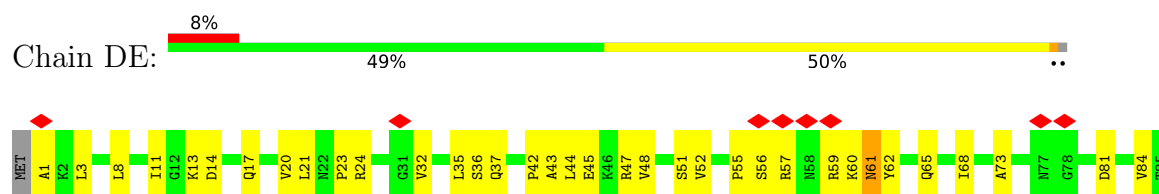
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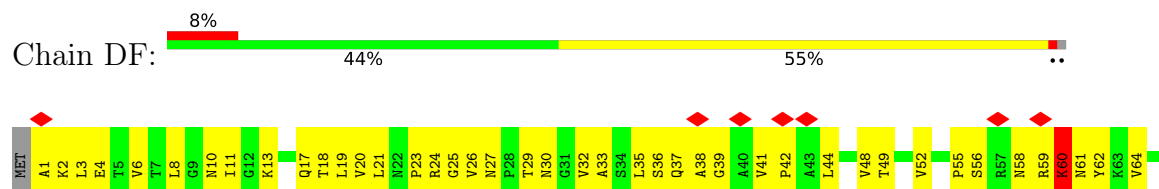
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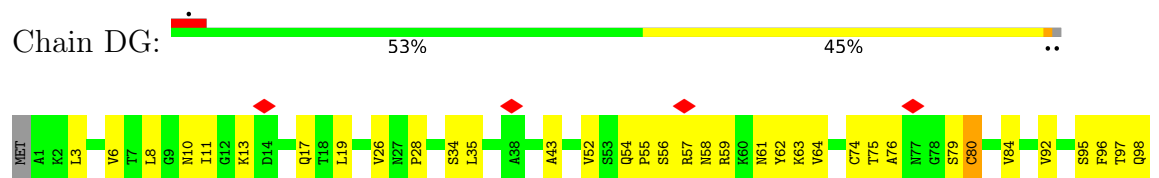
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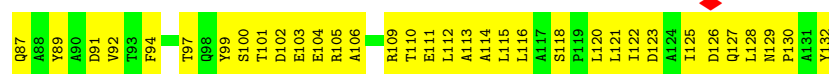
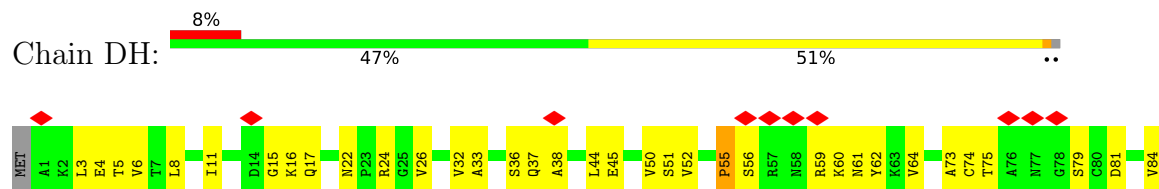
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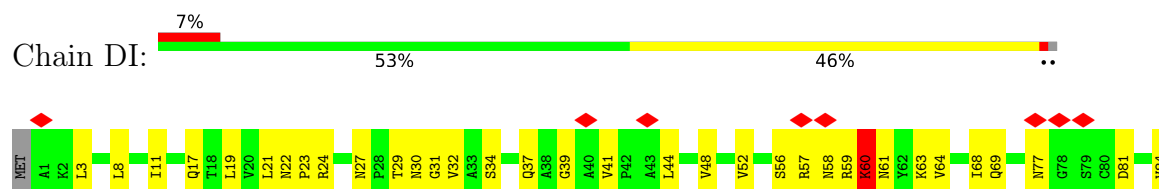
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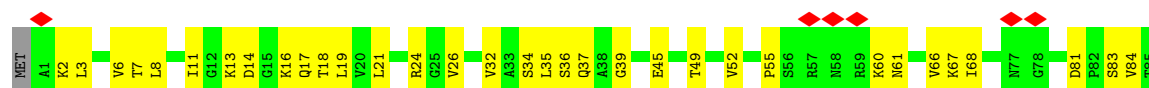




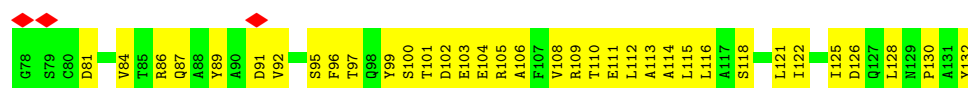
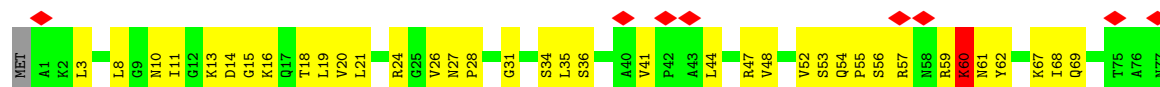
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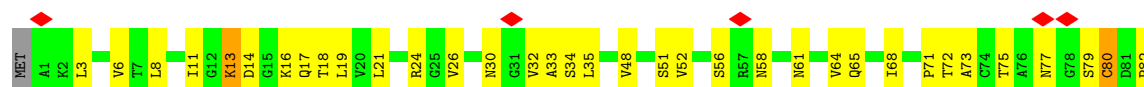
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- Molecule 3: Capsid protein

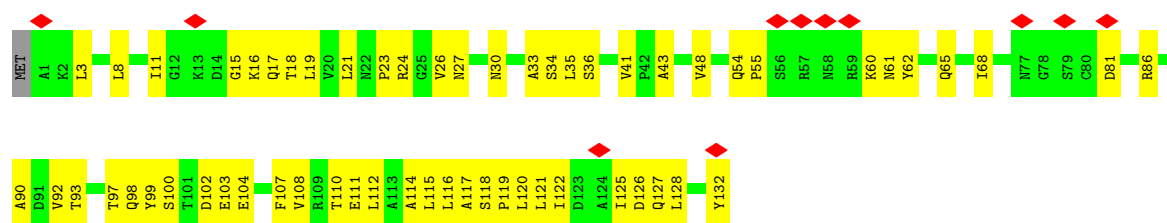


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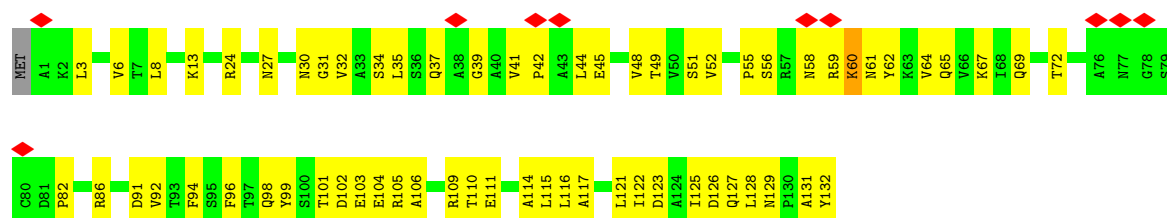
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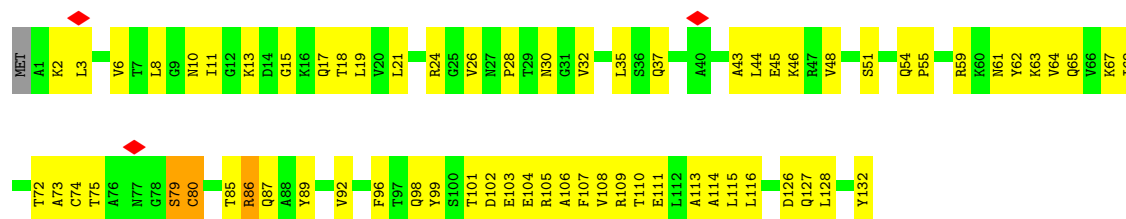
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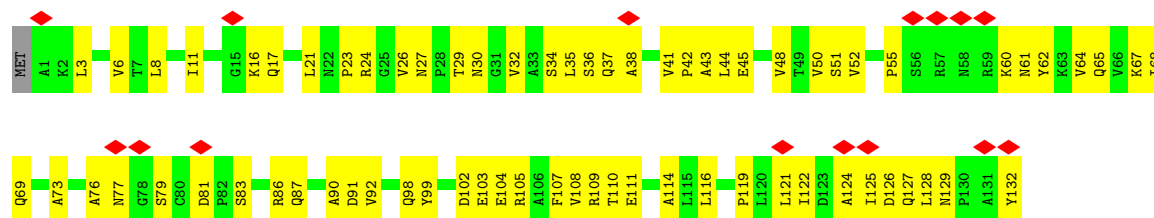
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• Molecule 3: Capsid protein

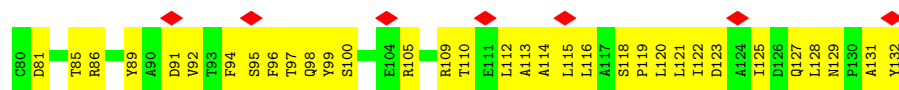
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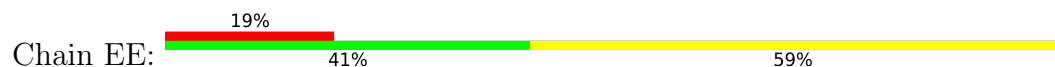
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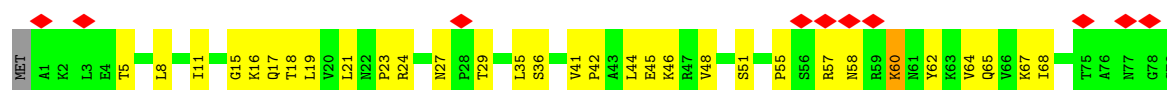




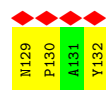
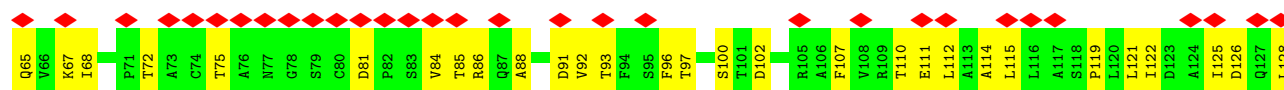
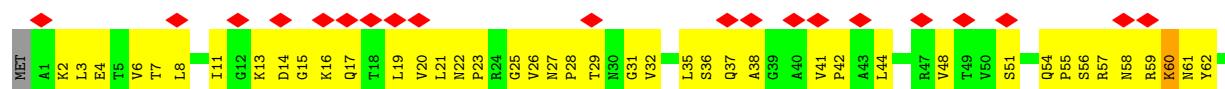
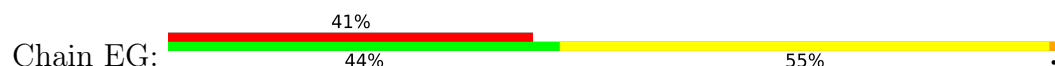
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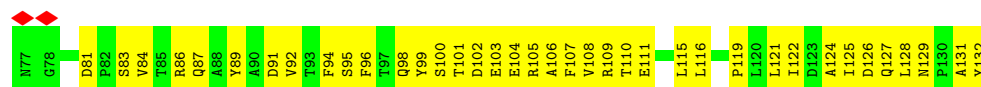
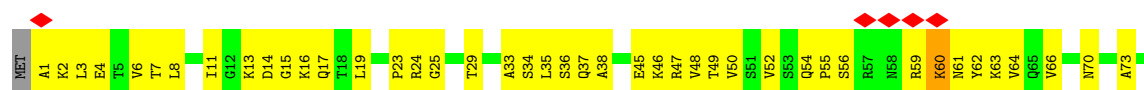


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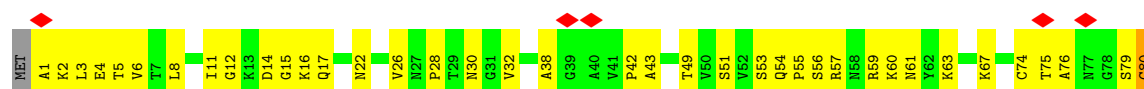
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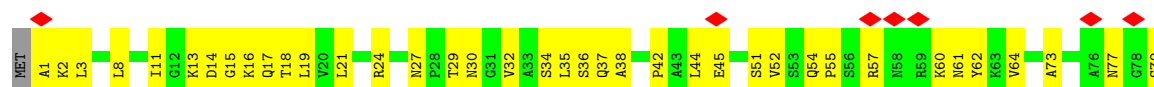
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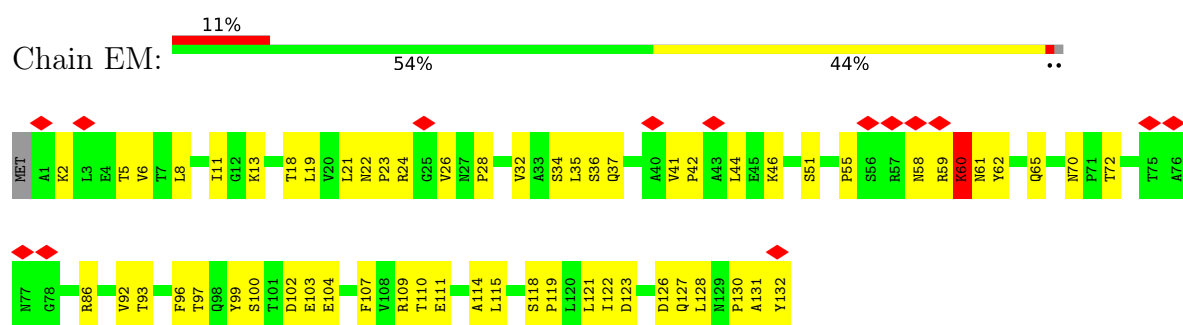
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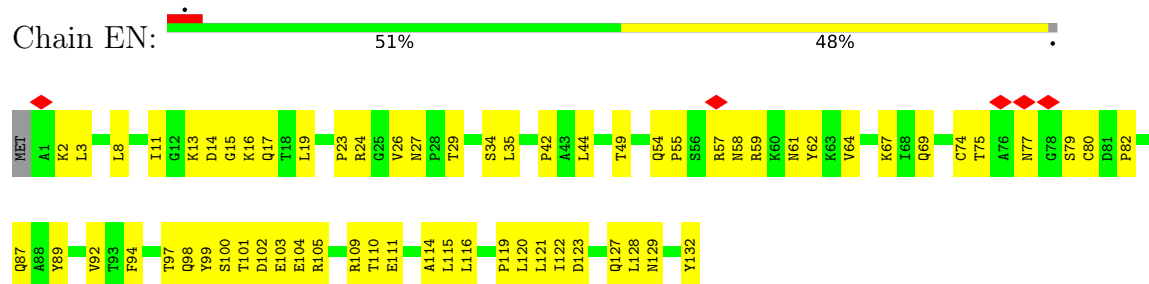
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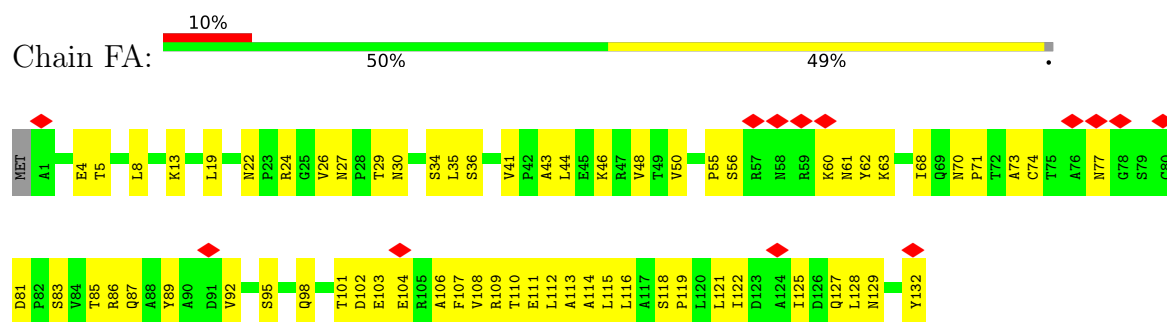
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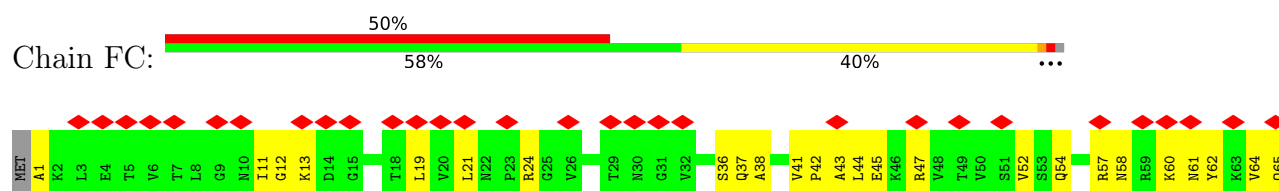
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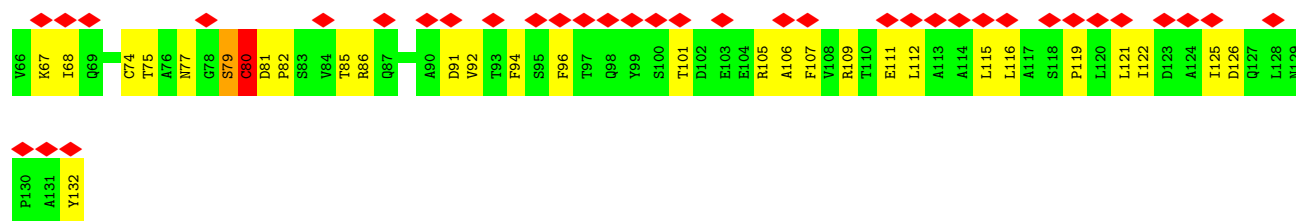


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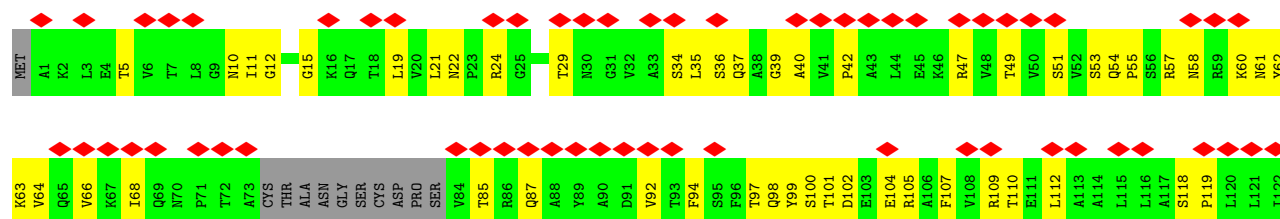


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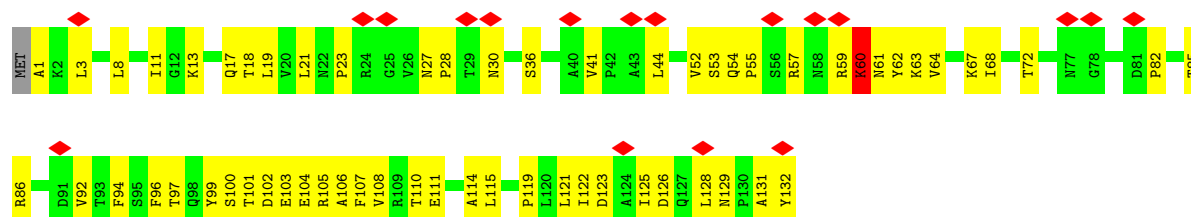




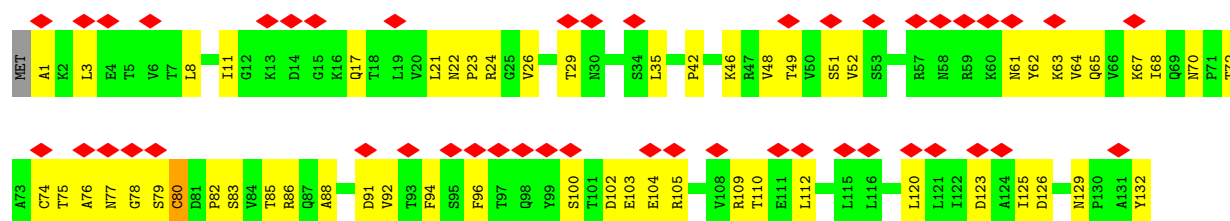
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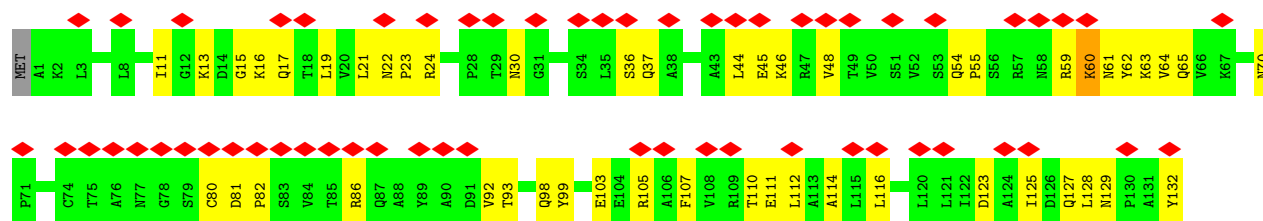


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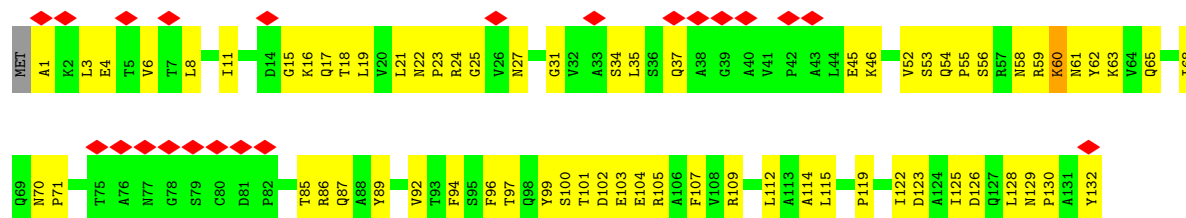


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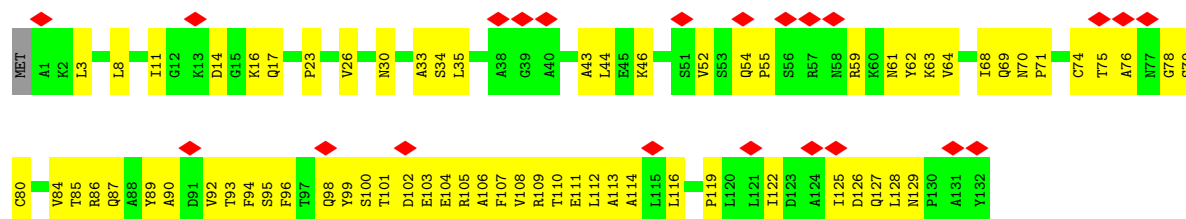




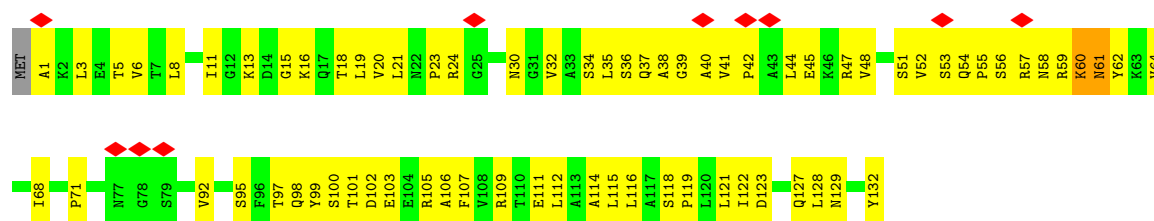
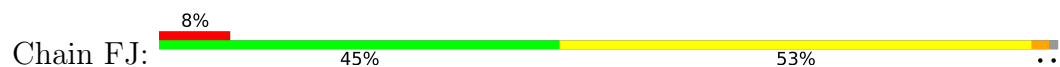
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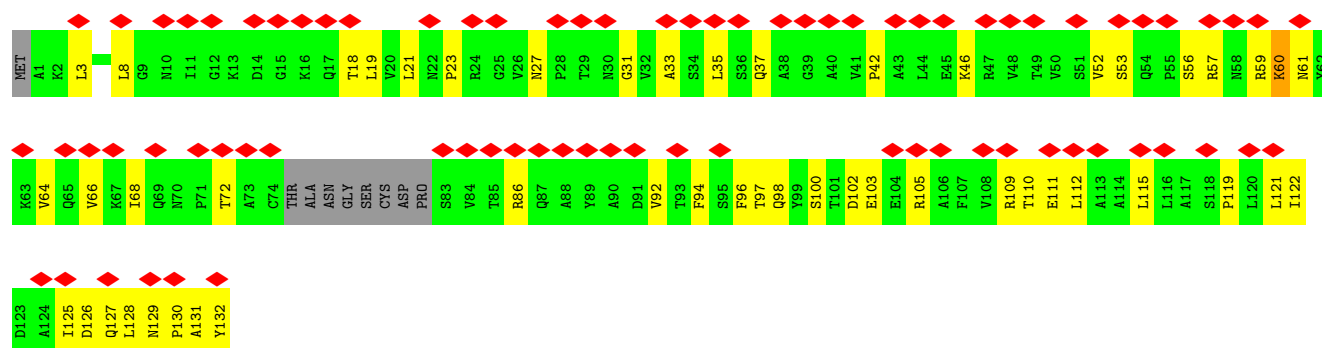


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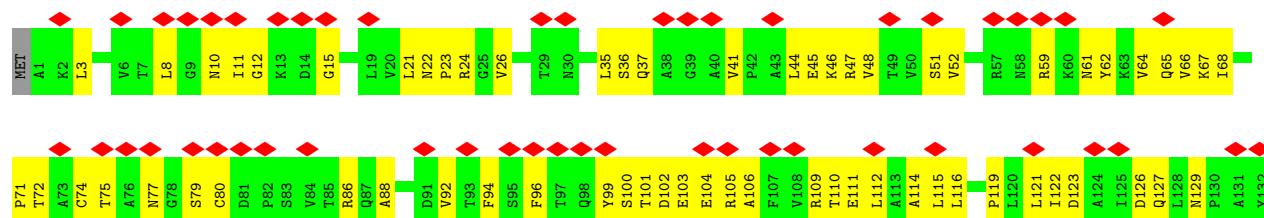
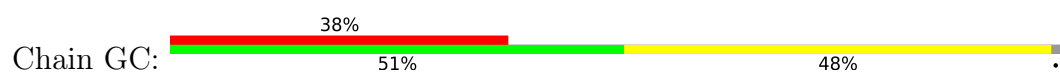


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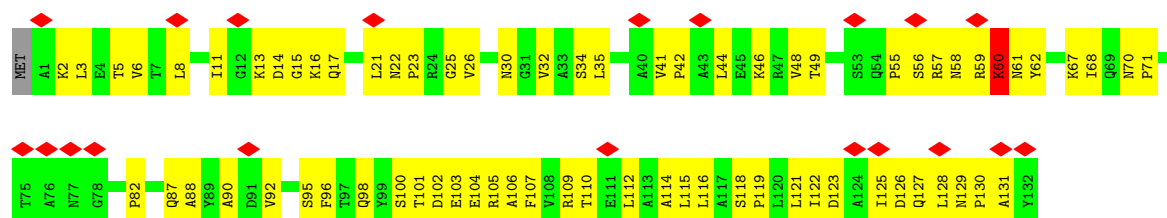




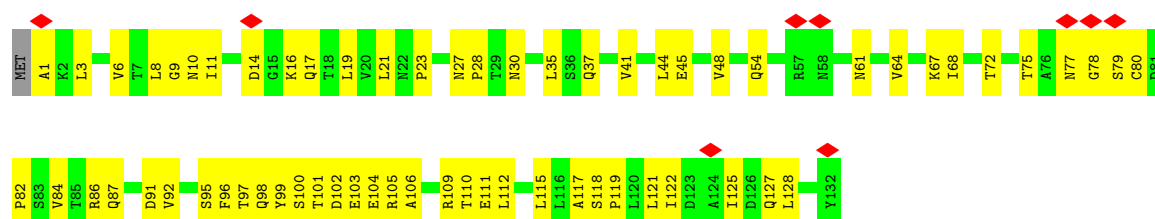
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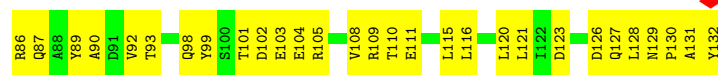
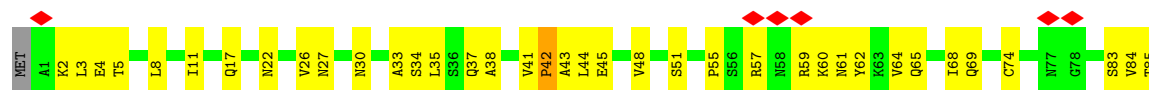


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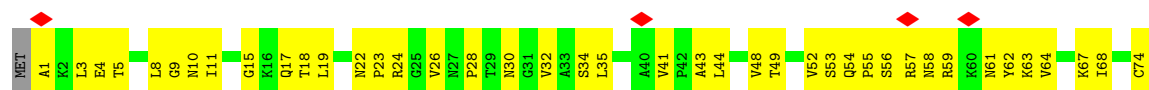
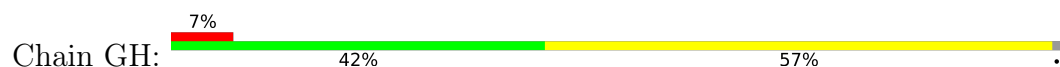




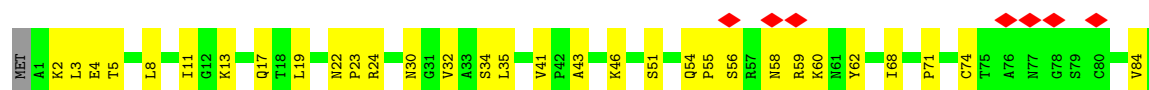
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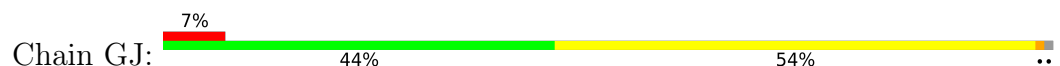
• Molecule 3: Capsid protein



• Molecule 3: Capsid protein

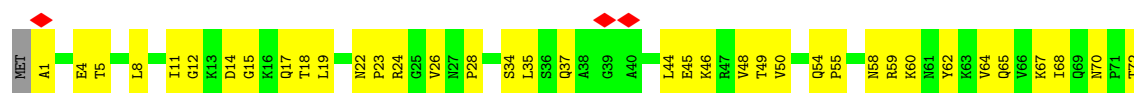
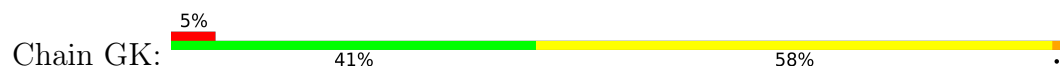


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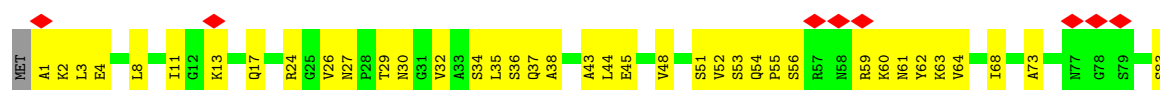




- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



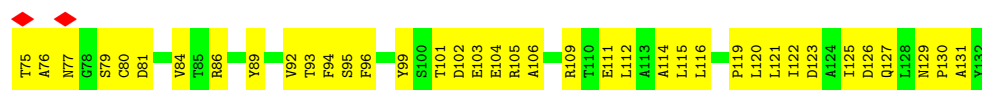
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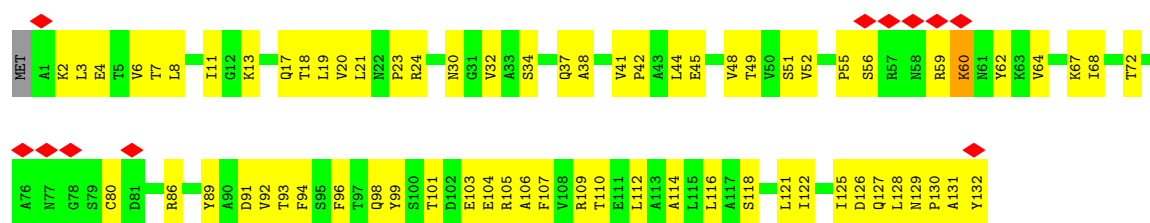


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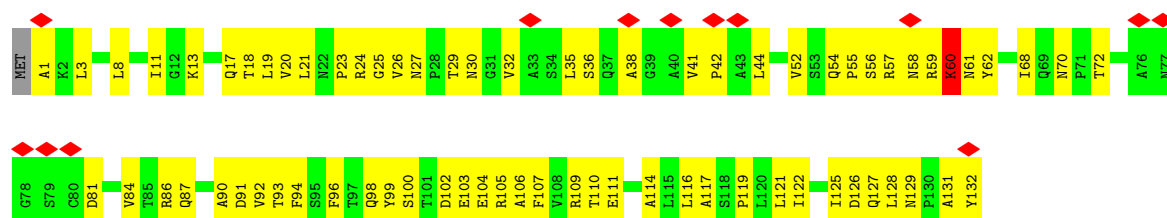


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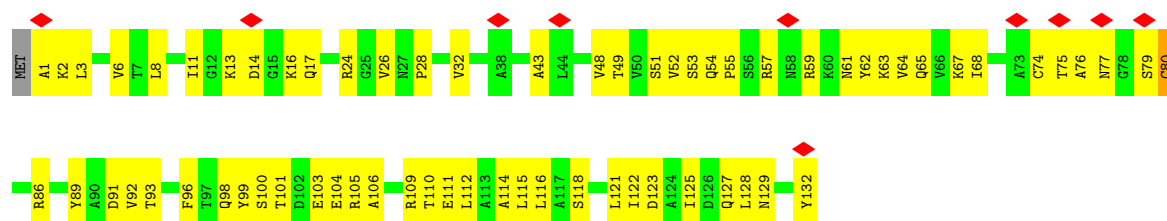




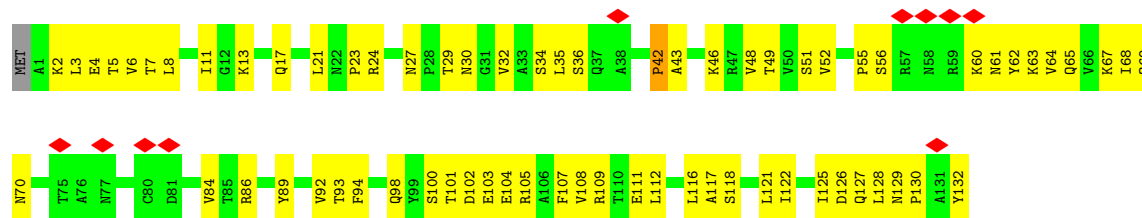
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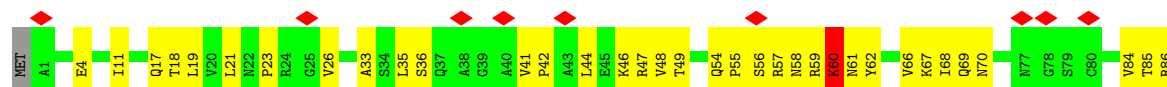
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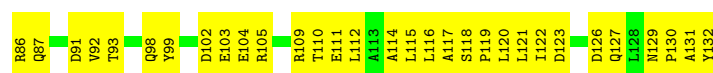
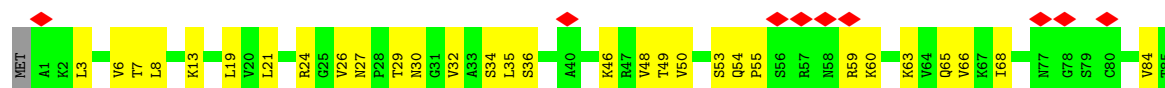




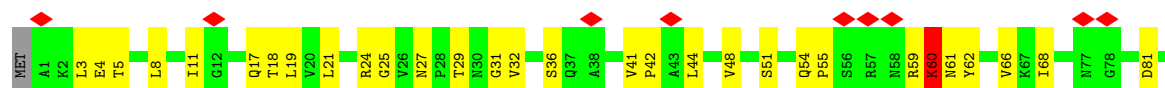
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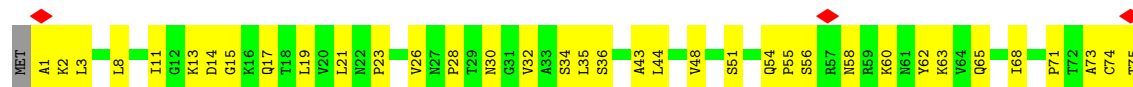
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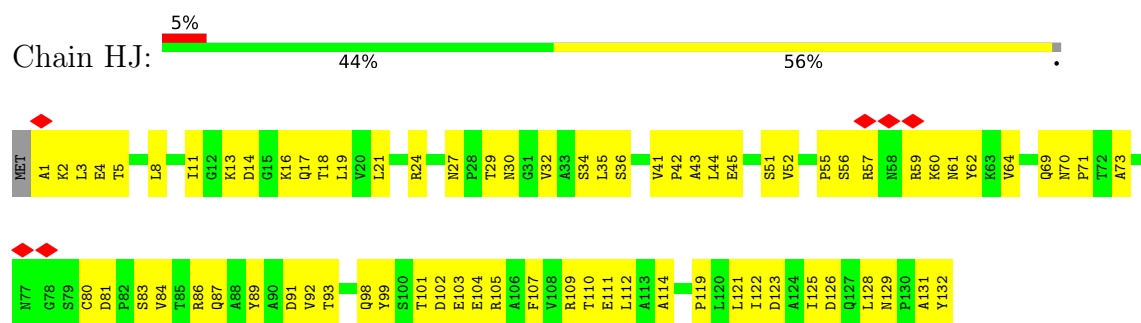
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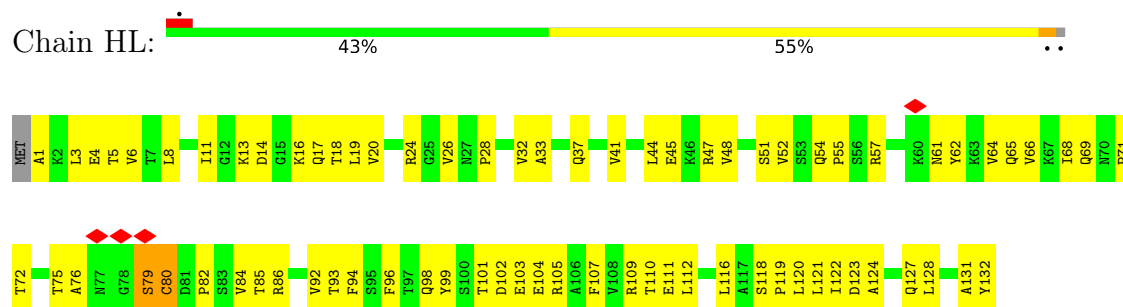
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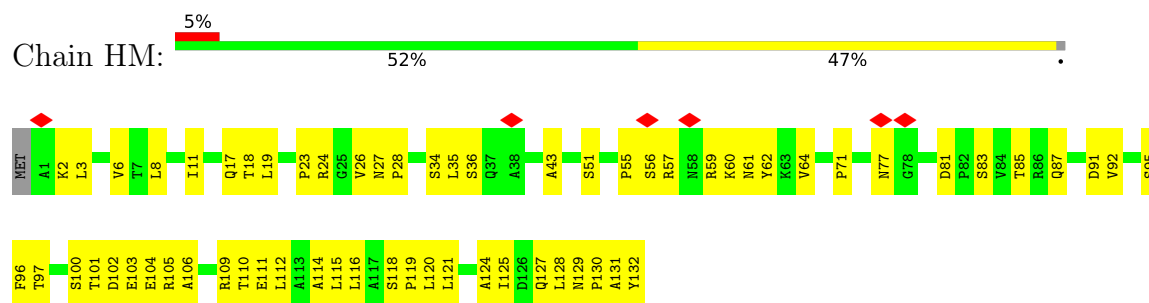
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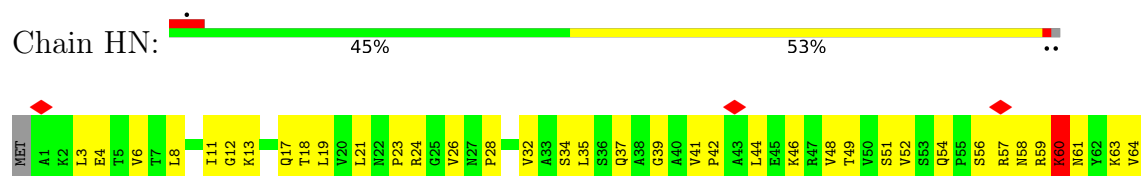
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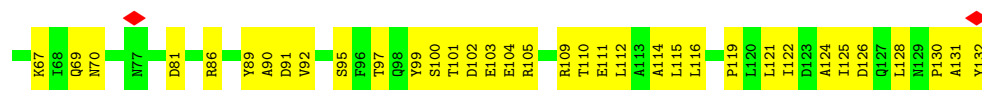


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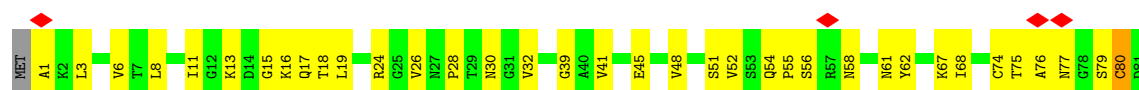


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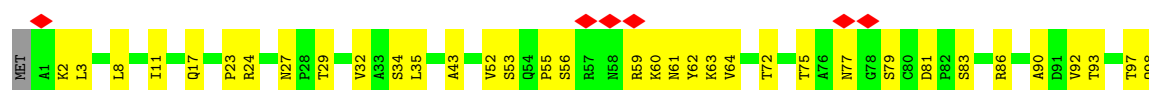




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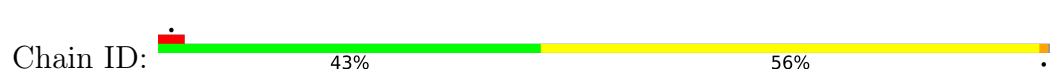
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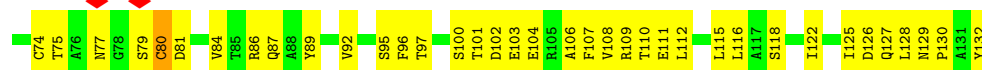
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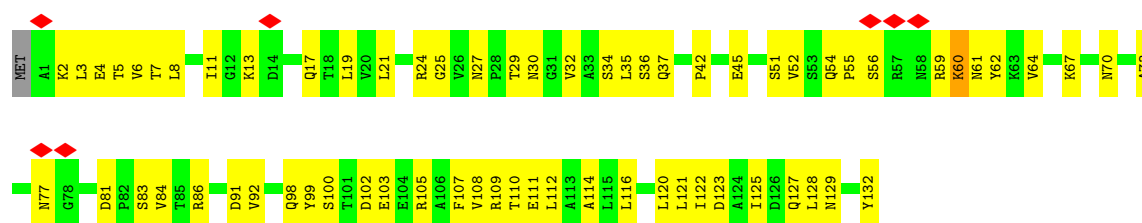


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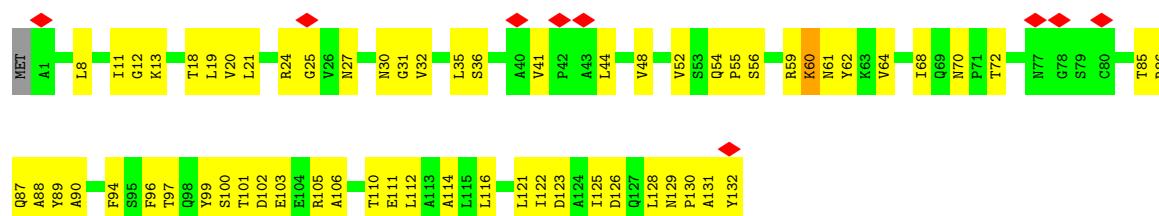


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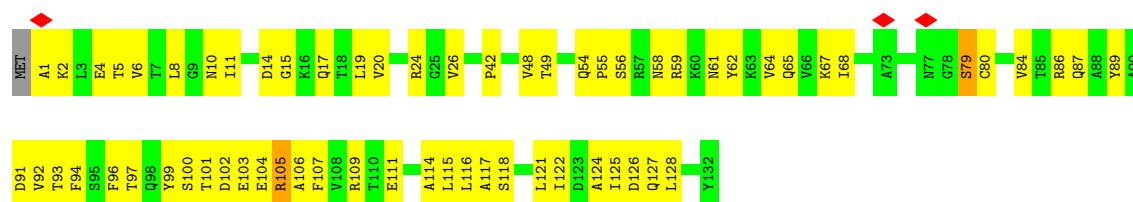




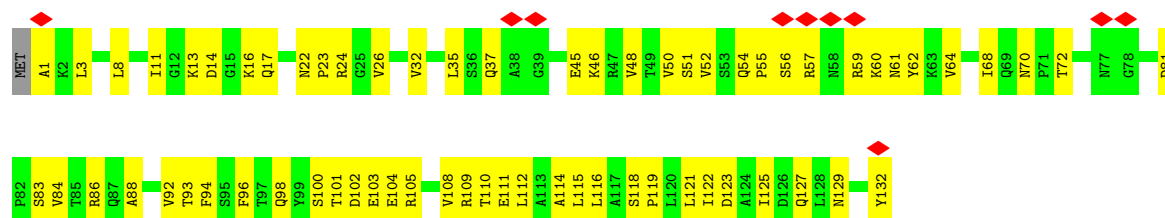
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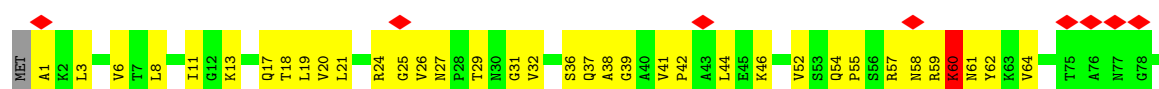
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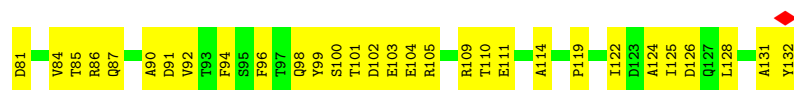


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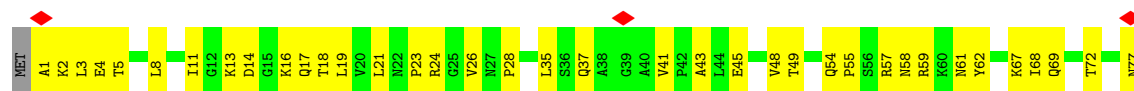


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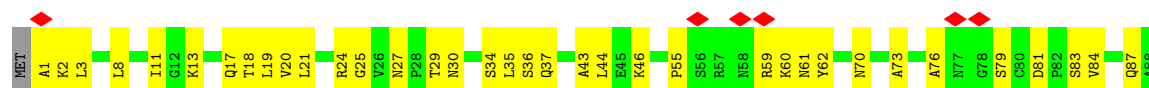




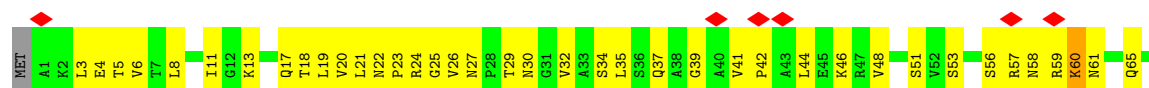
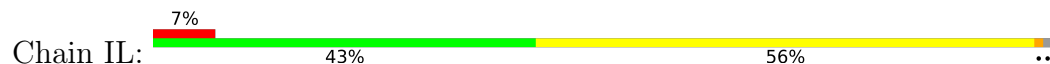
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- Molecule 3: Capsid protein



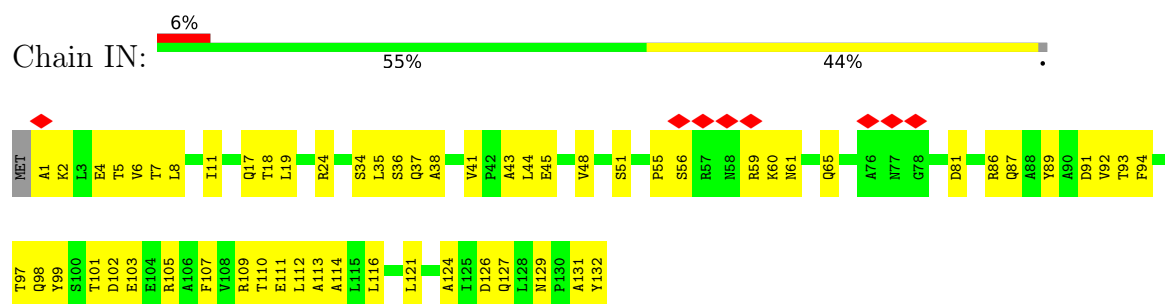
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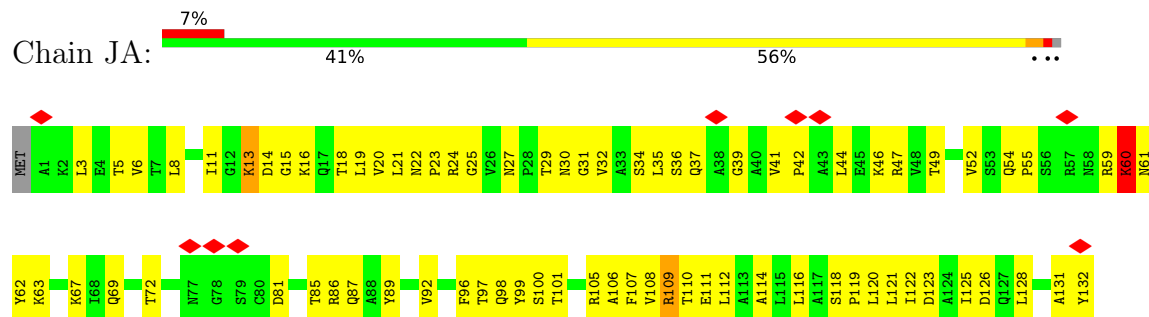
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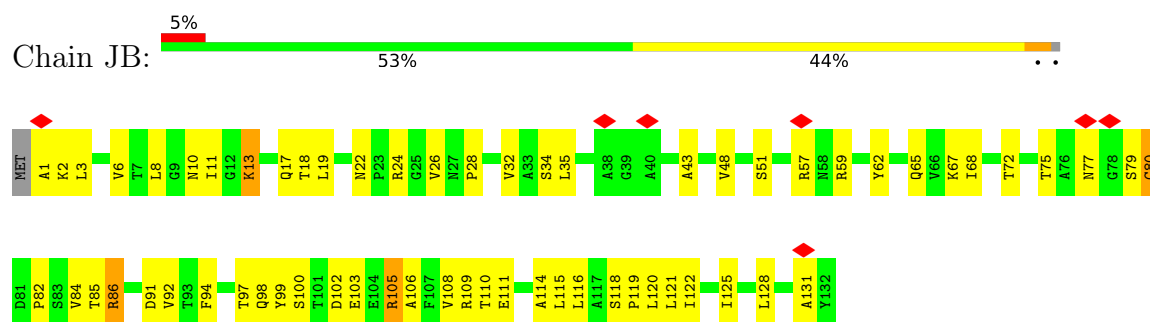
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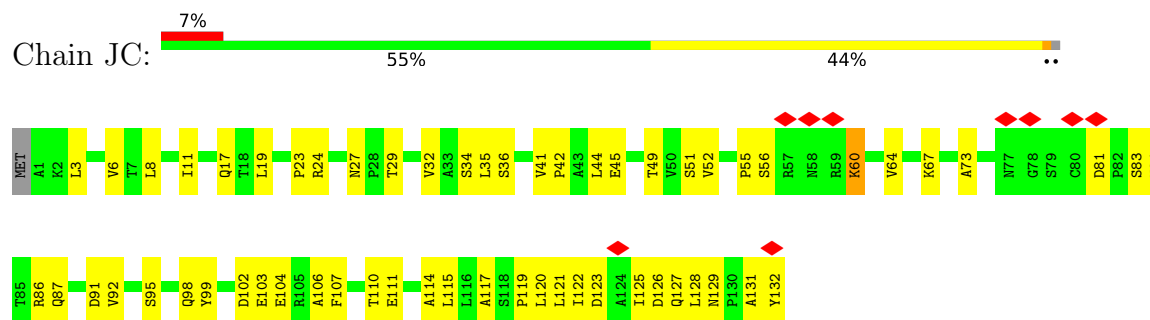
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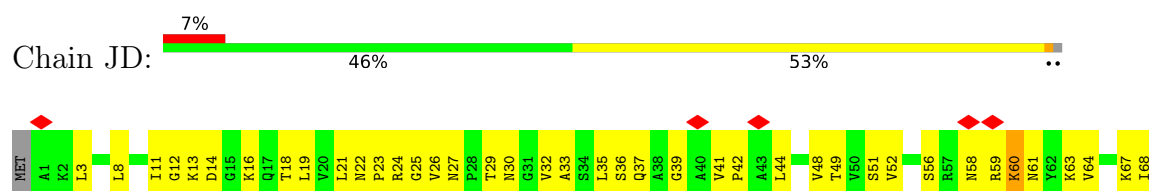
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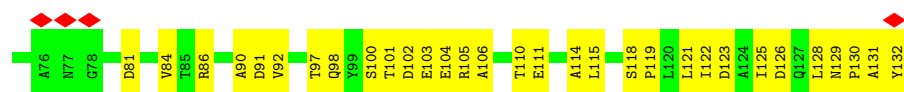


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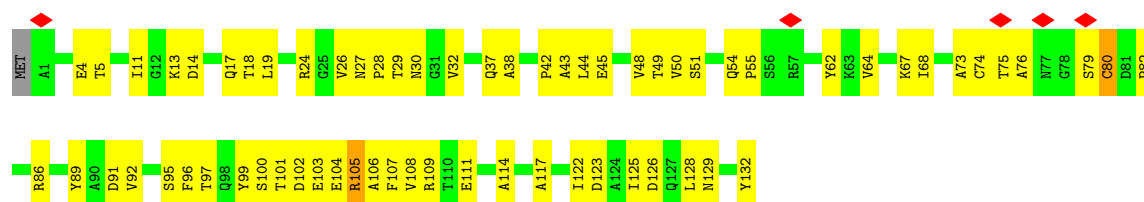


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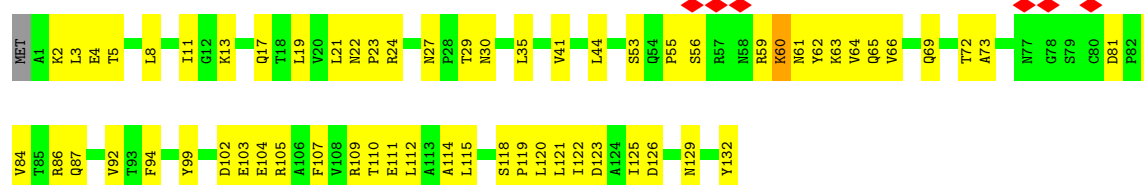




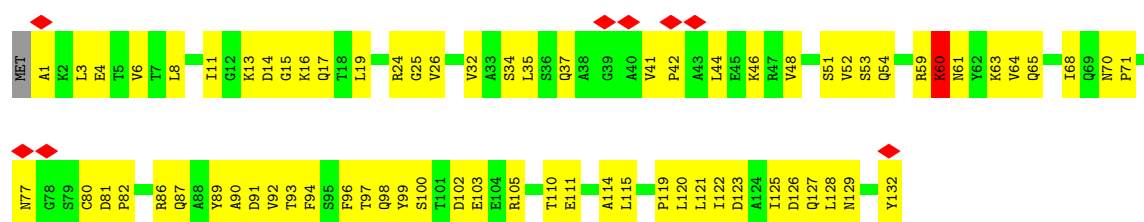
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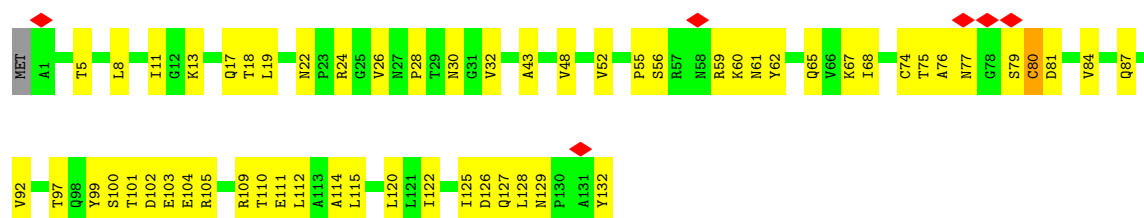
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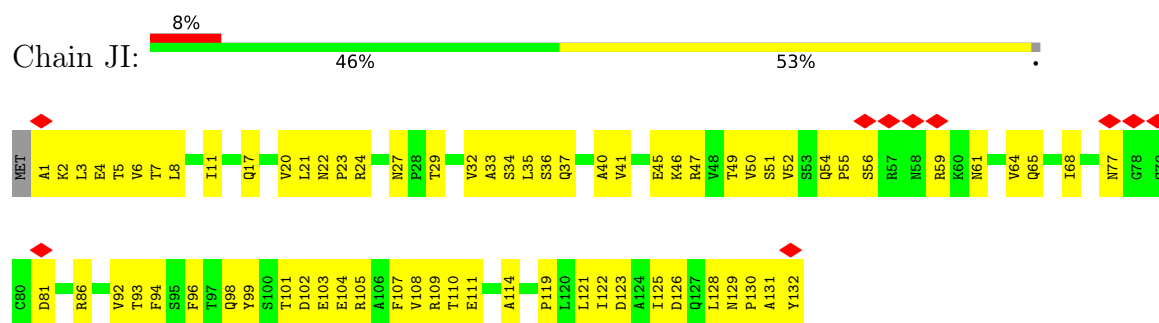
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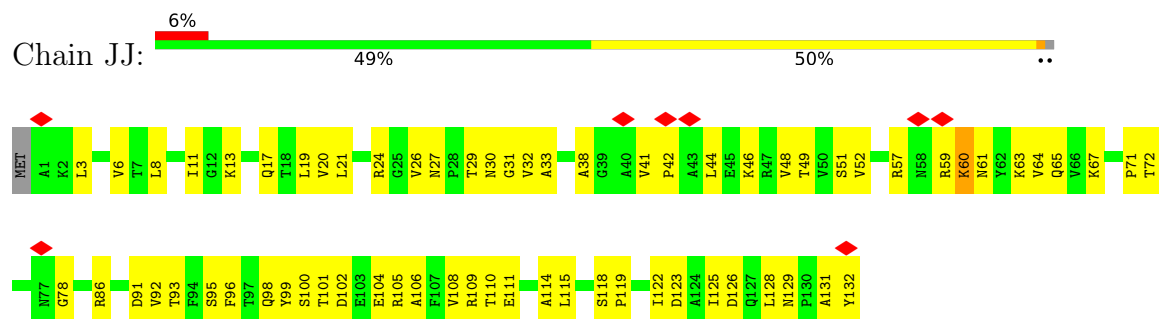
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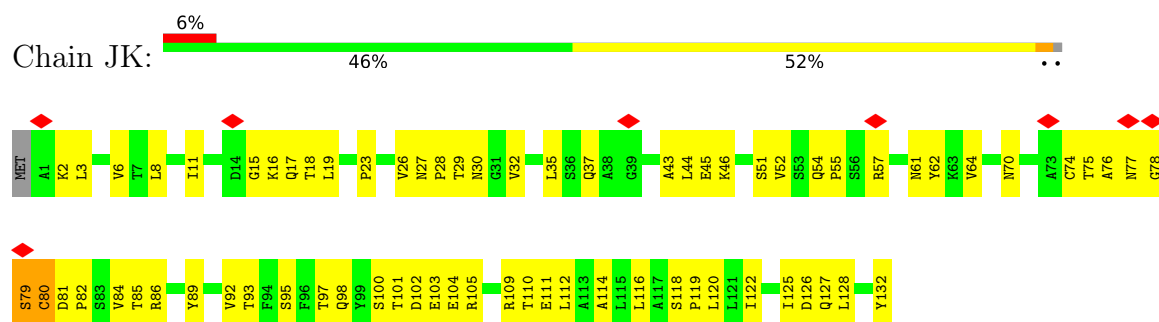
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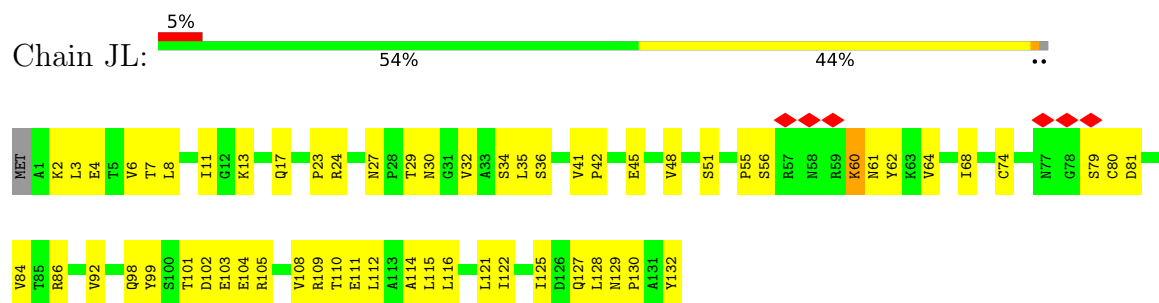
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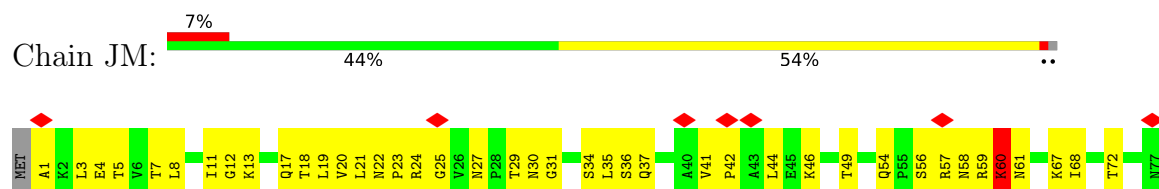
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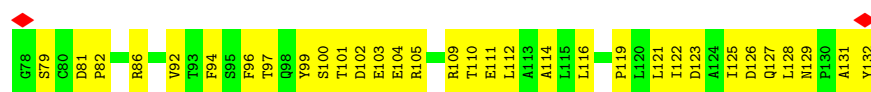


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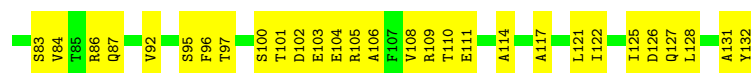


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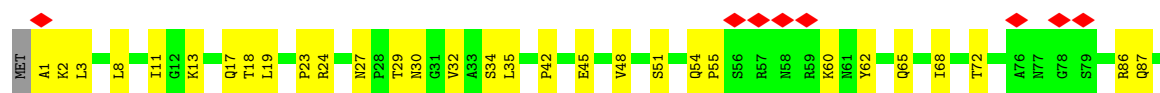




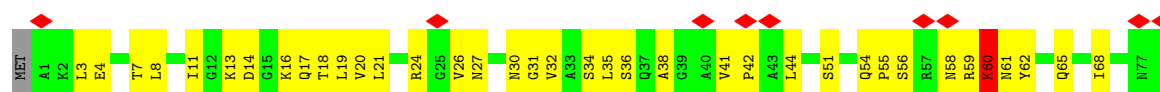
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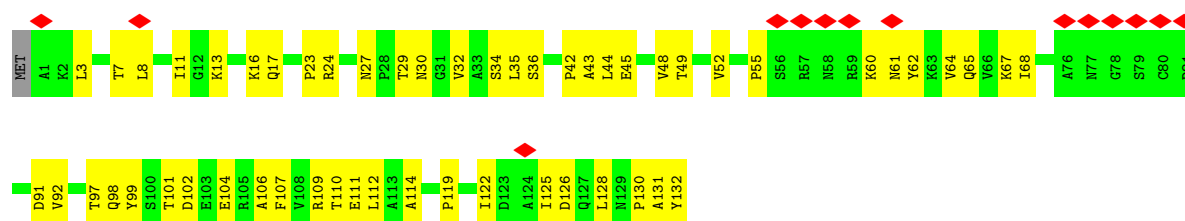


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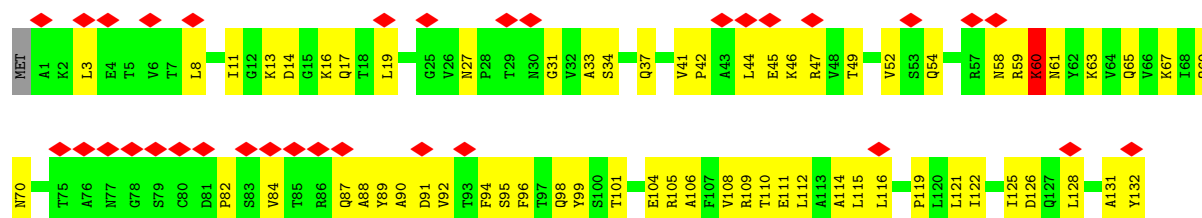
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Chain KD: 11% 59% 41%



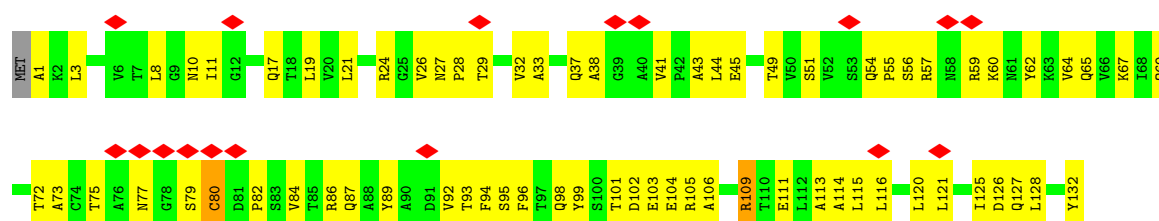
• Molecule 3: Capsid protein

Chain KE: 25% 51% 47%



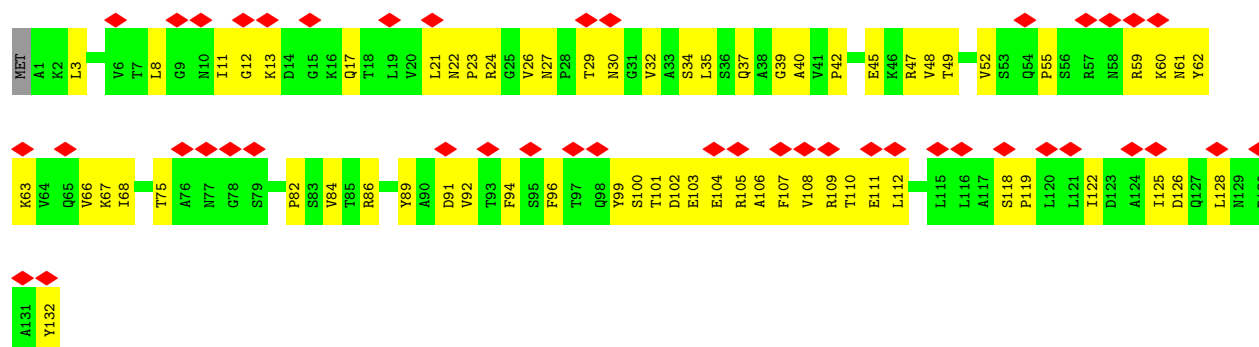
• Molecule 3: Capsid protein

Chain KF: 13% 46% 52%



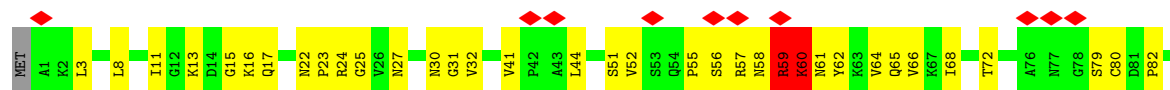
• Molecule 3: Capsid protein

Chain KG: 33% 50% 49%

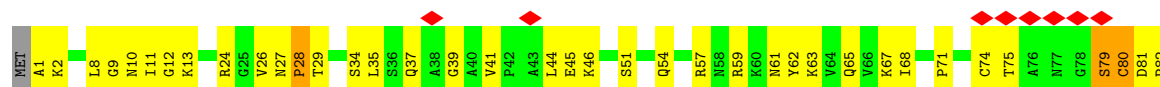


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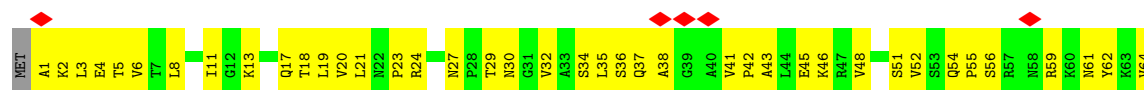
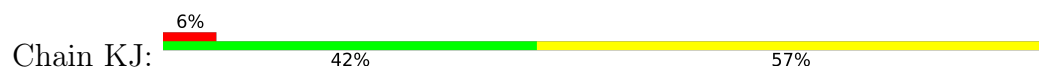
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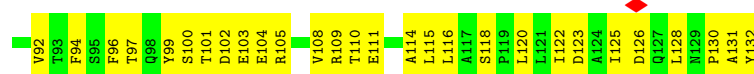
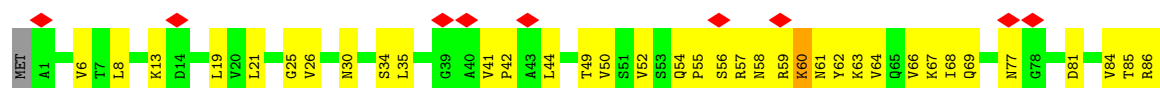
• Molecule 3: Capsid protein



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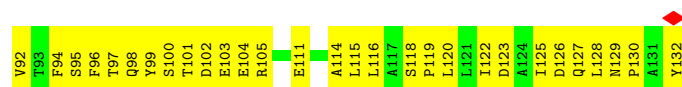
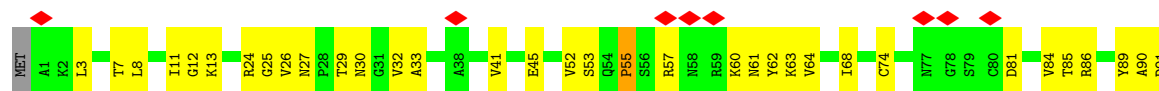


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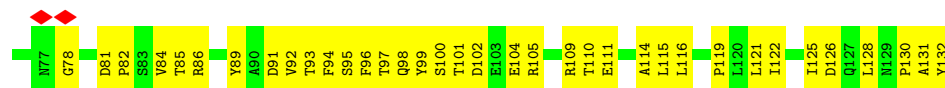
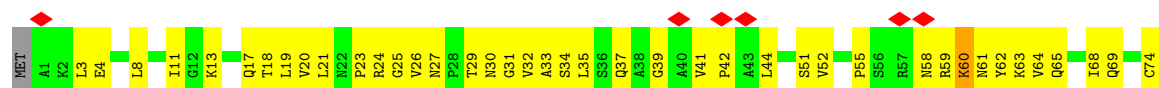
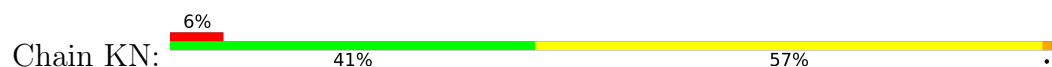




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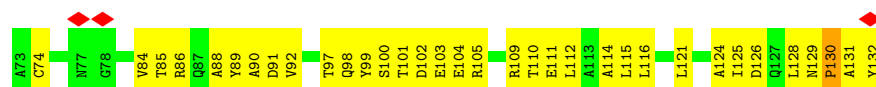
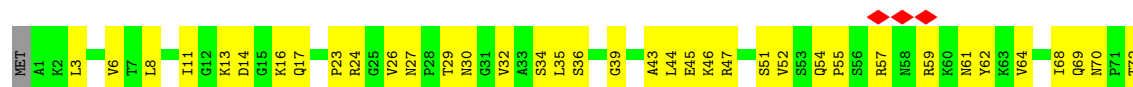
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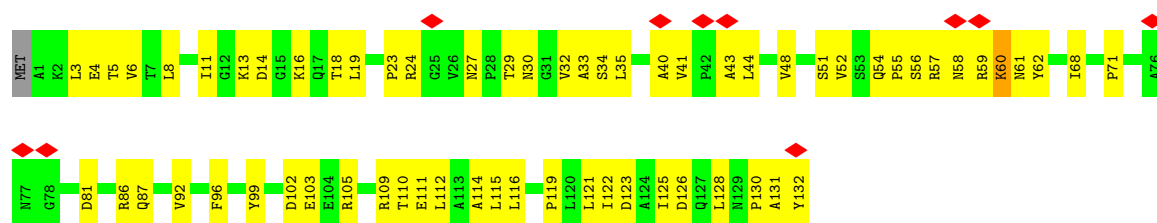
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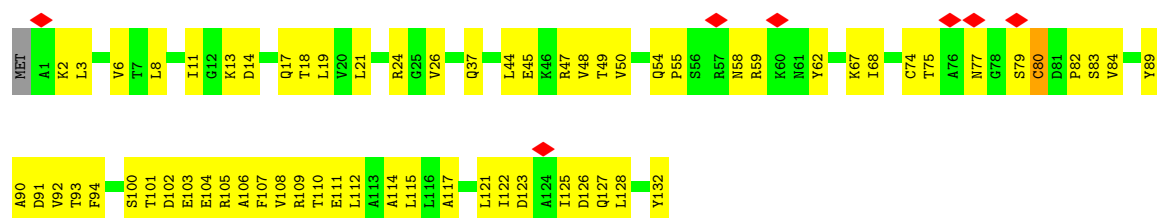
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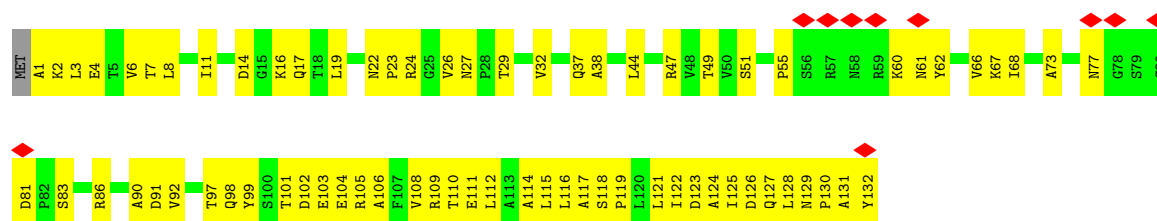
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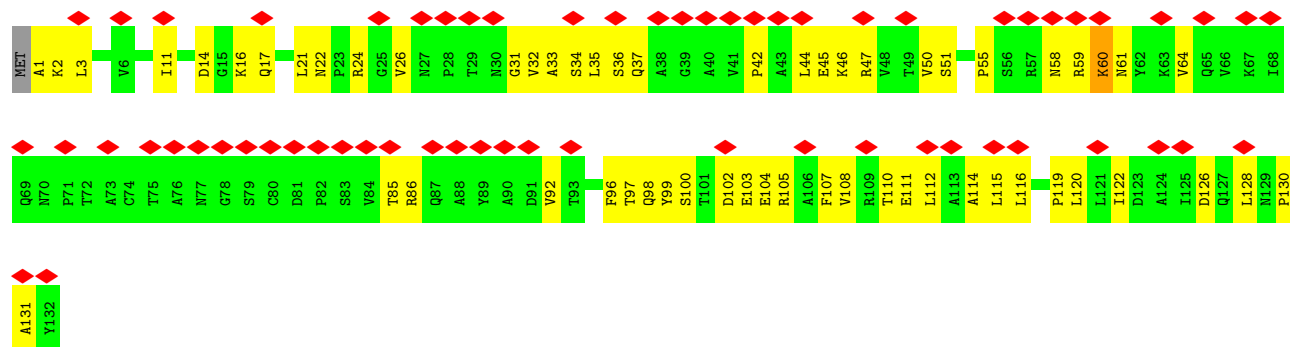
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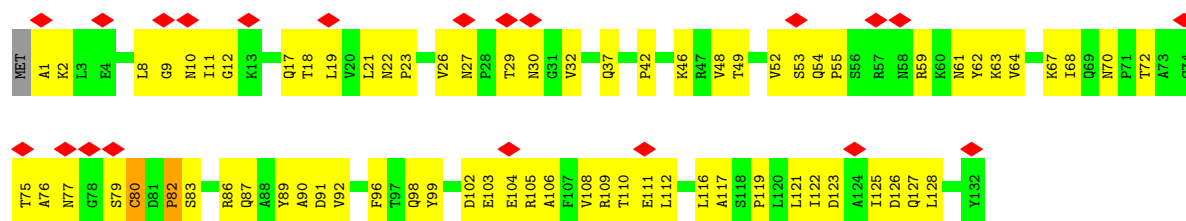


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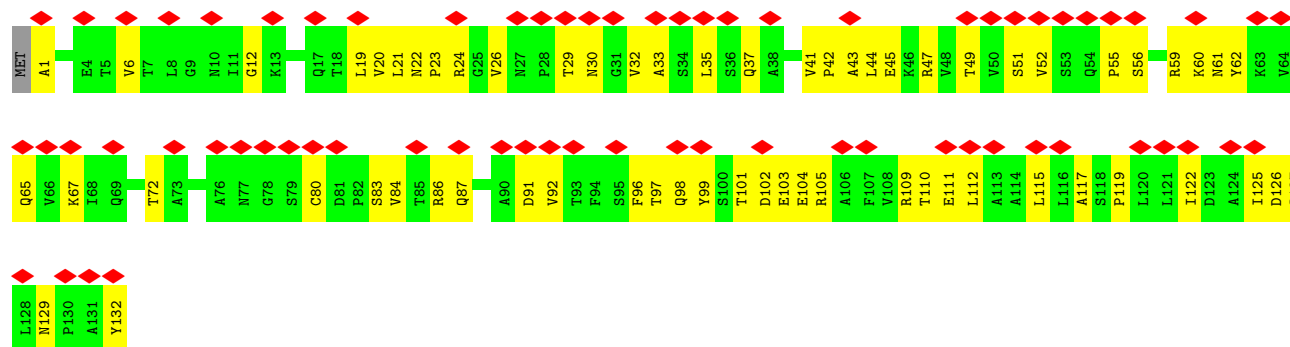


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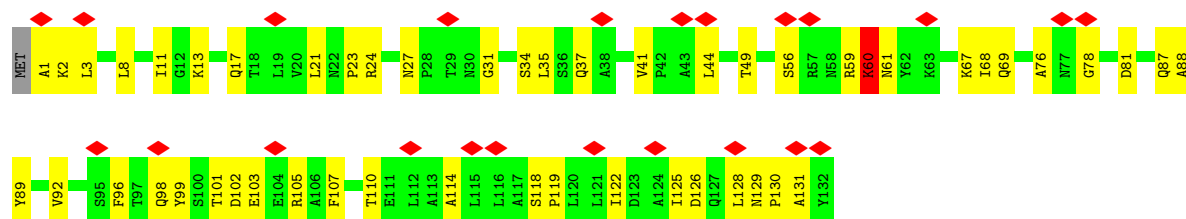




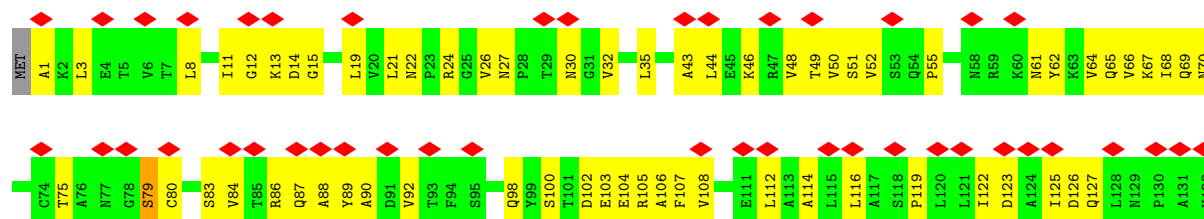
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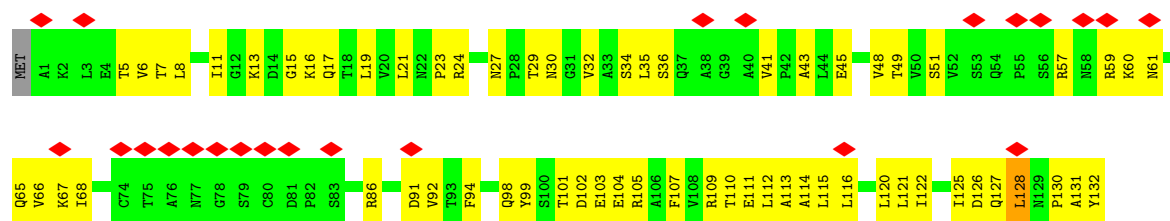


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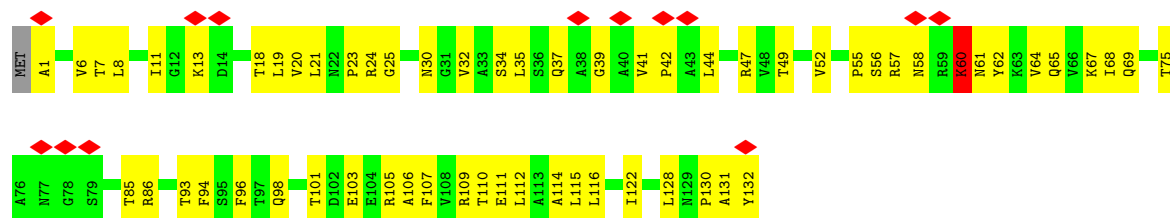


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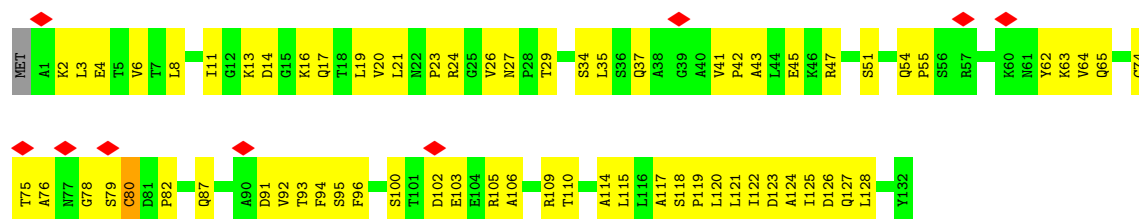




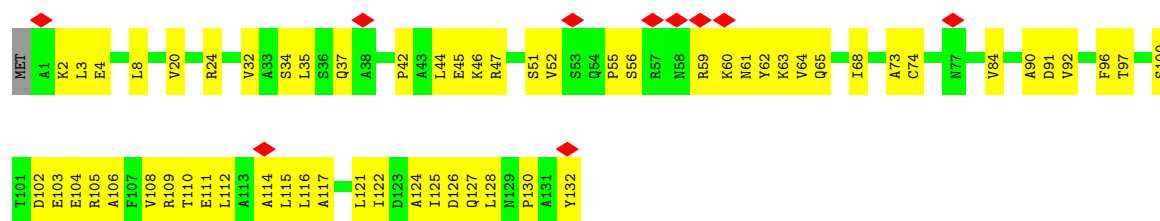
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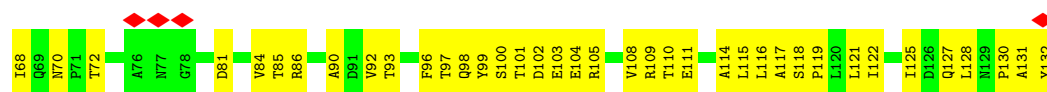


- Molecule 3: Capsid protein



- Molecule 3: Capsid protein

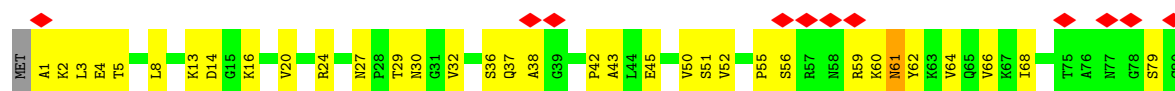




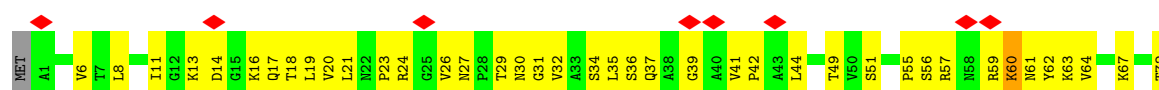
- Molecule 3: Capsid protein



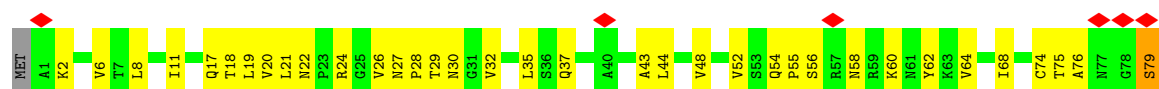
- Molecule 3: Capsid protein



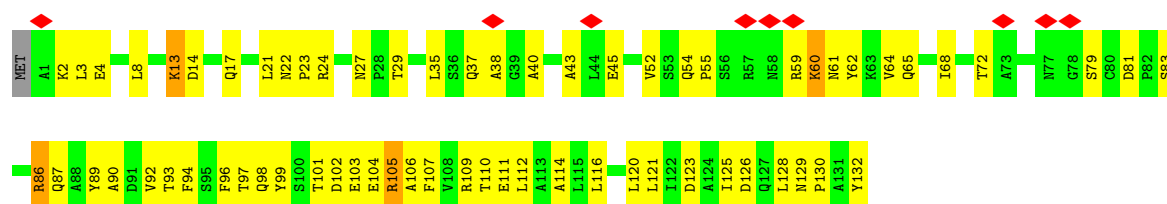
- Molecule 3: Capsid protein



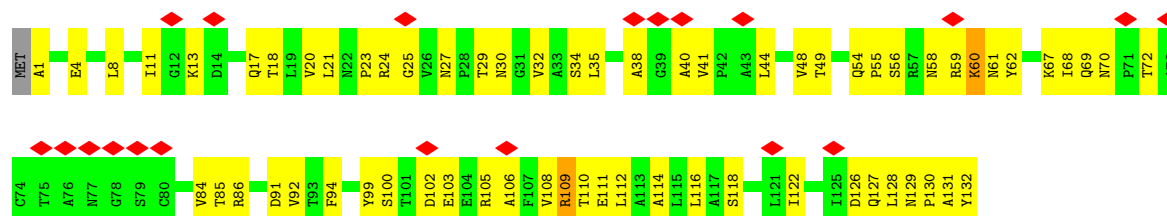
- Molecule 3: Capsid protein



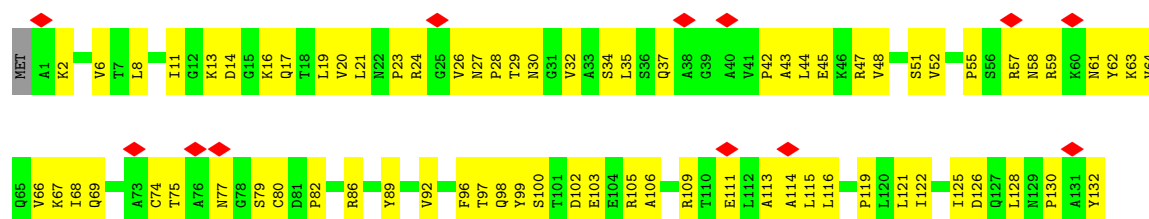
- Molecule 3: Capsid protein



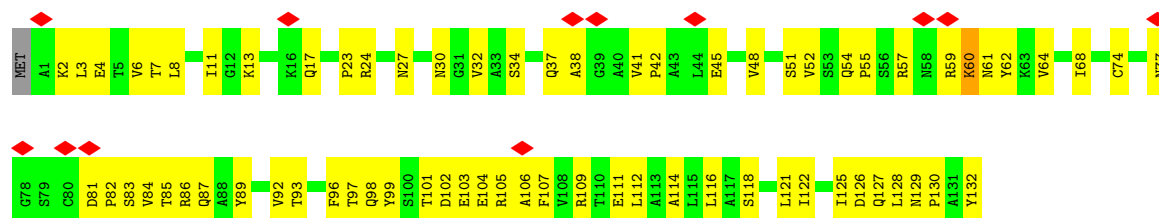
- Molecule 3: Capsid protein



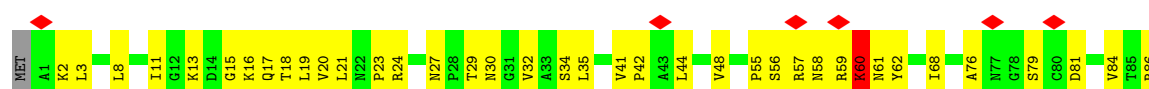
- Molecule 3: Capsid protein

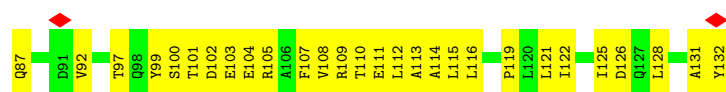


- Molecule 3: Capsid protein

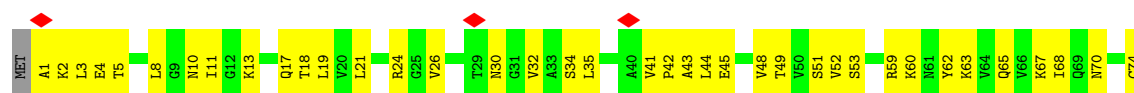


- Molecule 3: Capsid protein

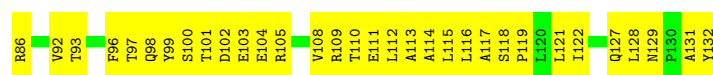
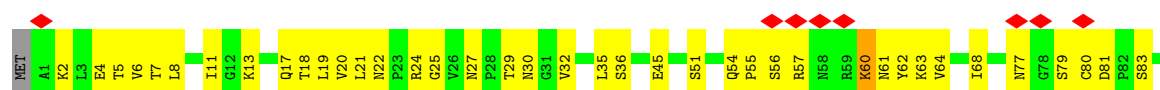




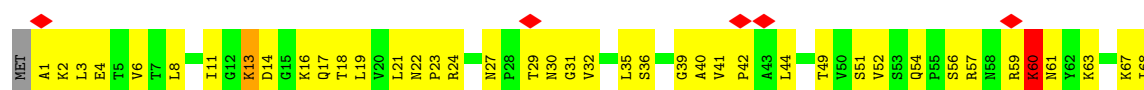
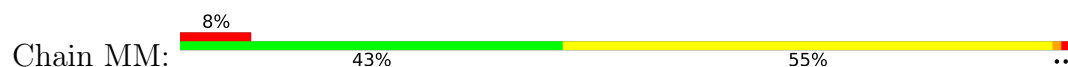
- Molecule 3: Capsid protein



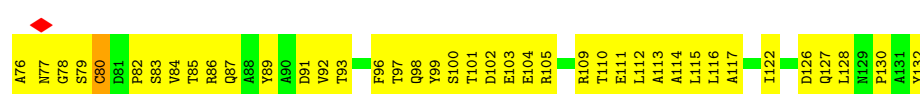
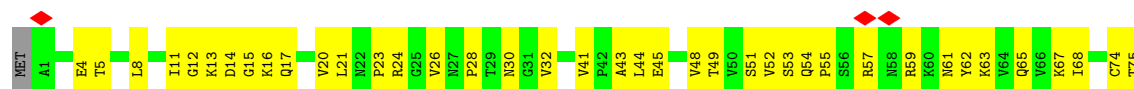
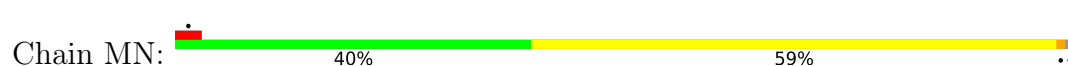
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



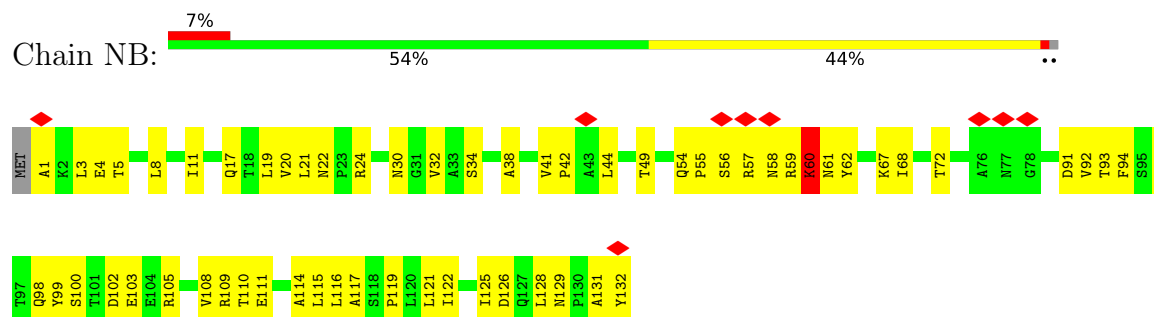
- Molecule 3: Capsid protein



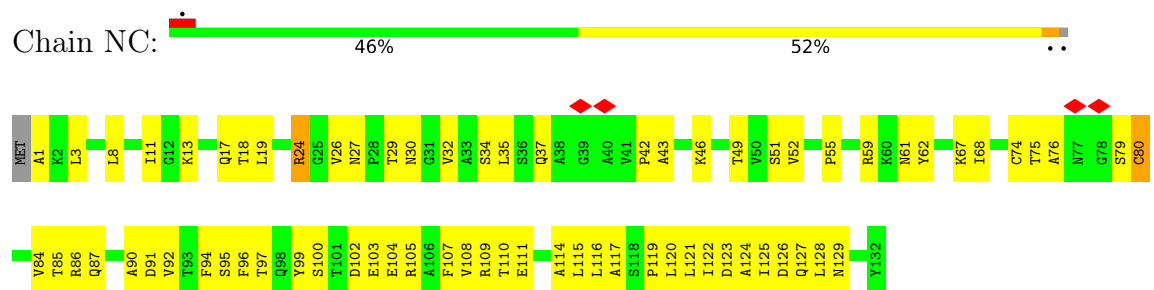
- Molecule 3: Capsid protein



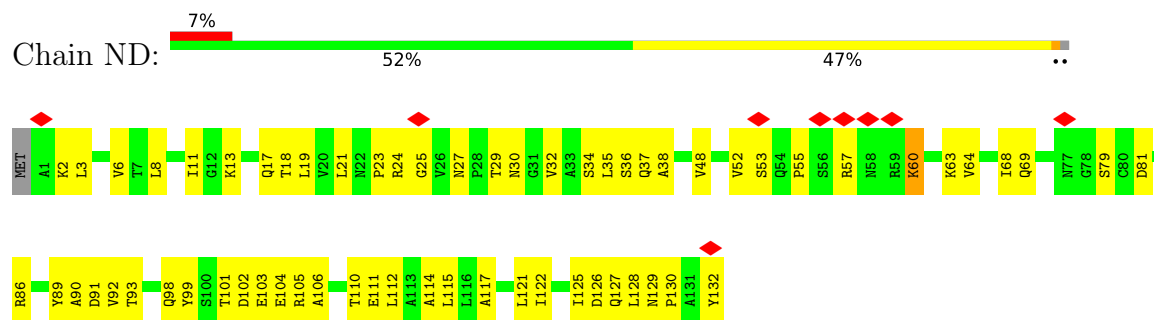
- Molecule 3: Capsid protein



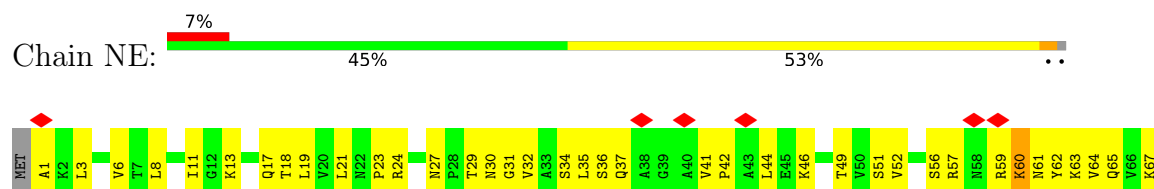
- Molecule 3: Capsid protein

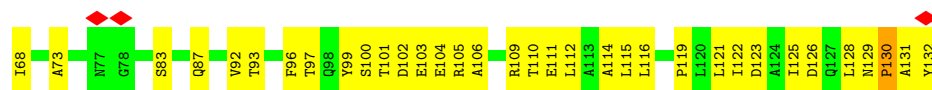


- Molecule 3: Capsid protein

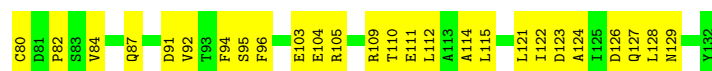


- Molecule 3: Capsid protein





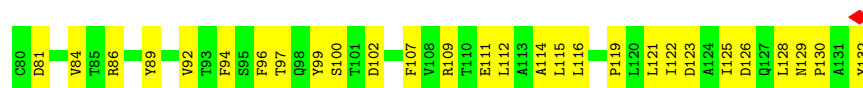
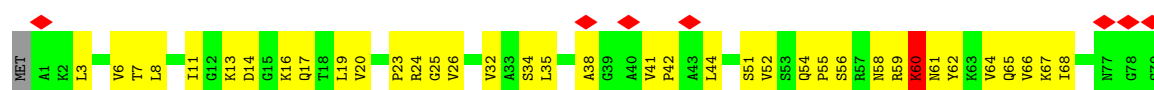
- Molecule 3: Capsid protein



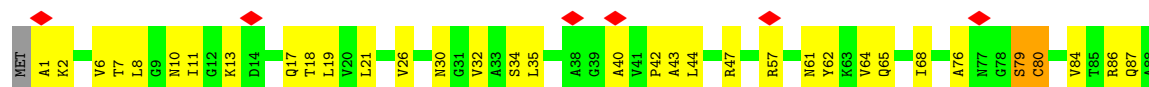
- Molecule 3: Capsid protein



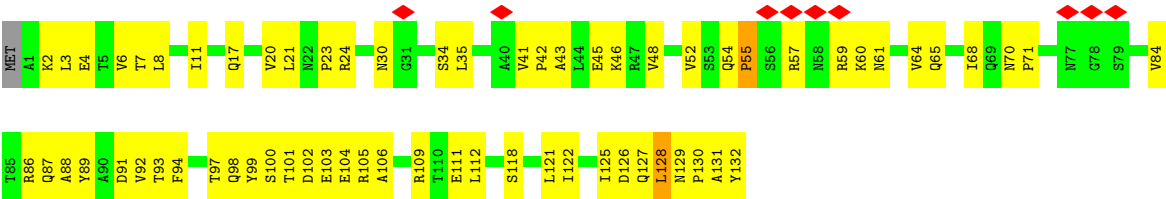
- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



- Molecule 3: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86081	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC, FEI TECNAI F20	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30, 30	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/99732	0.34	0/155312
2	M	0.25	0/3532	0.44	1/4790 (0.0%)
3	B	0.23	0/1007	0.42	0/1371
3	BA	0.40	0/1007	0.65	2/1371 (0.1%)
3	BB	0.46	0/1007	0.67	1/1371 (0.1%)
3	BC	0.40	0/1007	0.47	0/1371
3	BD	0.43	0/1007	0.68	2/1371 (0.1%)
3	BE	0.39	0/1007	0.54	0/1371
3	BF	0.42	0/1007	0.61	0/1371
3	BG	0.39	0/1007	0.61	3/1371 (0.2%)
3	BH	0.42	0/1007	0.68	2/1371 (0.1%)
3	BI	0.41	0/1007	0.55	0/1371
3	BJ	0.44	0/1007	0.67	3/1371 (0.2%)
3	BK	0.42	0/1007	0.54	0/1371
3	BL	0.41	0/1007	0.52	0/1371
3	BM	0.38	0/1007	0.61	2/1371 (0.1%)
3	BN	0.40	0/1007	0.56	0/1371
3	CA	0.41	0/1007	0.55	0/1371
3	CB	0.41	0/1007	0.71	4/1371 (0.3%)
3	CC	0.47	0/1007	0.62	2/1371 (0.1%)
3	CD	0.39	0/1007	0.57	1/1371 (0.1%)
3	CE	0.45	0/1007	0.65	3/1371 (0.2%)
3	CF	0.40	0/1007	0.56	0/1371
3	CG	0.43	0/1007	0.66	1/1371 (0.1%)
3	CH	0.40	0/1007	0.65	3/1371 (0.2%)
3	CI	0.39	0/1007	0.53	0/1371
3	CJ	0.42	0/1007	0.62	2/1371 (0.1%)
3	CK	0.39	0/1007	0.58	2/1371 (0.1%)
3	CL	0.43	0/1007	0.59	0/1371
3	CM	0.40	0/1007	0.58	1/1371 (0.1%)
3	CN	0.41	0/1007	0.59	3/1371 (0.2%)
3	D	0.23	0/1007	0.49	2/1371 (0.1%)
3	DA	0.40	0/1007	0.58	0/1371
3	DB	0.45	0/1007	0.62	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	DC	0.37	0/1007	0.61	2/1371 (0.1%)
3	DD	0.43	0/1007	0.59	0/1371
3	DE	0.43	0/1007	0.59	0/1371
3	DF	0.45	0/1007	0.63	3/1371 (0.2%)
3	DG	0.45	0/1007	0.62	0/1371
3	DH	0.47	1/1007 (0.1%)	0.63	3/1371 (0.2%)
3	DI	0.38	0/1007	0.56	2/1371 (0.1%)
3	DJ	0.41	0/1007	0.57	0/1371
3	DK	0.41	0/1007	0.59	0/1371
3	DL	0.40	0/1007	0.61	3/1371 (0.2%)
3	DM	0.42	0/1007	0.66	1/1371 (0.1%)
3	DN	0.37	0/1007	0.51	0/1371
3	EA	0.38	0/1007	0.65	2/1371 (0.1%)
3	EB	0.42	0/1007	0.61	1/1371 (0.1%)
3	EC	0.37	0/1007	0.57	0/1371
3	ED	0.33	0/1007	0.62	2/1371 (0.1%)
3	EE	0.36	0/1007	0.61	0/1371
3	EF	0.38	0/1007	0.54	0/1371
3	EG	0.32	0/1007	0.57	2/1371 (0.1%)
3	EH	0.39	1/1007 (0.1%)	0.60	2/1371 (0.1%)
3	EI	0.43	0/1007	0.57	0/1371
3	EJ	0.46	0/1007	0.72	3/1371 (0.2%)
3	EK	0.38	0/1007	0.59	2/1371 (0.1%)
3	EL	0.43	0/1007	0.53	0/1371
3	EM	0.39	0/1007	0.62	2/1371 (0.1%)
3	EN	0.41	0/1007	0.51	0/1371
3	FA	0.37	0/1007	0.57	0/1371
3	FB	0.34	0/1007	0.62	3/1371 (0.2%)
3	FC	0.28	0/1007	0.55	1/1371 (0.1%)
3	FD	0.28	0/942	0.51	0/1280
3	FE	0.34	0/1007	0.63	2/1371 (0.1%)
3	FF	0.33	0/1007	0.54	0/1371
3	FG	0.31	0/1007	0.53	0/1371
3	FH	0.37	0/1007	0.62	2/1371 (0.1%)
3	FI	0.39	0/1007	0.55	0/1371
3	FJ	0.41	0/1007	0.66	2/1371 (0.1%)
3	FK	0.43	0/1007	0.65	0/1371
3	FL	0.38	0/1007	0.56	0/1371
3	FM	0.40	0/1007	0.61	2/1371 (0.1%)
3	FN	0.41	0/1007	0.65	2/1371 (0.1%)
3	GA	0.37	0/1007	0.53	0/1371
3	GB	0.24	0/954	0.52	3/1296 (0.2%)
3	GC	0.34	0/1007	0.58	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	GD	0.38	0/1007	0.67	2/1371 (0.1%)
3	GE	0.39	0/1007	0.52	0/1371
3	GF	0.38	0/1007	0.54	1/1371 (0.1%)
3	GG	0.44	0/1007	0.68	2/1371 (0.1%)
3	GH	0.42	0/1007	0.61	0/1371
3	GI	0.41	0/1007	0.51	0/1371
3	GJ	0.42	0/1007	0.65	2/1371 (0.1%)
3	GK	0.45	0/1007	0.61	0/1371
3	GL	0.40	0/1007	0.54	0/1371
3	GM	0.43	0/1007	0.71	2/1371 (0.1%)
3	GN	0.44	0/1007	0.60	0/1371
3	HA	0.39	0/1007	0.53	0/1371
3	HB	0.39	0/1007	0.58	2/1371 (0.1%)
3	HC	0.40	0/1007	0.55	0/1371
3	HD	0.43	1/1007 (0.1%)	0.63	2/1371 (0.1%)
3	HE	0.40	0/1007	0.60	2/1371 (0.1%)
3	HF	0.41	0/1007	0.54	0/1371
3	HG	0.40	0/1007	0.53	0/1371
3	HH	0.38	0/1007	0.59	3/1371 (0.2%)
3	HI	0.42	0/1007	0.60	0/1371
3	HJ	0.42	0/1007	0.60	0/1371
3	HK	0.41	0/1007	0.64	2/1371 (0.1%)
3	HL	0.40	0/1007	0.59	0/1371
3	HM	0.44	0/1007	0.55	0/1371
3	HN	0.40	0/1007	0.59	3/1371 (0.2%)
3	IA	0.43	0/1007	0.59	0/1371
3	IB	0.43	0/1007	0.54	0/1371
3	IC	0.43	0/1007	0.63	2/1371 (0.1%)
3	ID	0.43	0/1007	0.58	0/1371
3	IE	0.45	0/1007	0.56	0/1371
3	IF	0.39	0/1007	0.60	2/1371 (0.1%)
3	IG	0.43	0/1007	0.60	1/1371 (0.1%)
3	IH	0.44	0/1007	0.56	0/1371
3	II	0.44	0/1007	0.62	3/1371 (0.2%)
3	IJ	0.44	0/1007	0.59	1/1371 (0.1%)
3	IK	0.41	0/1007	0.56	0/1371
3	IL	0.41	0/1007	0.65	3/1371 (0.2%)
3	IM	0.39	0/1007	0.53	1/1371 (0.1%)
3	IN	0.38	0/1007	0.50	0/1371
3	JA	0.45	0/1007	0.73	5/1371 (0.4%)
3	JB	0.44	0/1007	0.66	4/1371 (0.3%)
3	JC	0.40	0/1007	0.53	0/1371
3	JD	0.40	0/1007	0.62	2/1371 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	JE	0.44	0/1007	0.68	1/1371 (0.1%)
3	JF	0.40	0/1007	0.55	0/1371
3	JG	0.43	0/1007	0.69	2/1371 (0.1%)
3	JH	0.38	0/1007	0.54	0/1371
3	JI	0.39	0/1007	0.54	0/1371
3	JJ	0.46	0/1007	0.70	2/1371 (0.1%)
3	JK	0.41	0/1007	0.53	0/1371
3	JL	0.39	0/1007	0.50	0/1371
3	JM	0.38	0/1007	0.63	2/1371 (0.1%)
3	JN	0.45	0/1007	0.56	0/1371
3	KA	0.41	0/1007	0.53	0/1371
3	KB	0.41	0/1007	0.67	2/1371 (0.1%)
3	KC	0.37	0/1007	0.59	0/1371
3	KD	0.39	0/1007	0.55	0/1371
3	KE	0.34	0/1007	0.66	2/1371 (0.1%)
3	KF	0.48	0/1007	0.65	1/1371 (0.1%)
3	KG	0.29	0/1007	0.52	0/1371
3	KH	0.43	0/1007	0.69	2/1371 (0.1%)
3	KI	0.40	0/1007	0.63	1/1371 (0.1%)
3	KJ	0.36	0/1007	0.52	0/1371
3	KK	0.38	0/1007	0.63	2/1371 (0.1%)
3	KL	0.40	0/1007	0.56	0/1371
3	KM	0.38	0/1007	0.58	1/1371 (0.1%)
3	KN	0.43	0/1007	0.62	2/1371 (0.1%)
3	LA	0.48	1/1007 (0.1%)	0.63	0/1371
3	LB	0.42	0/1007	0.61	1/1371 (0.1%)
3	LC	0.51	1/1007 (0.1%)	0.73	5/1371 (0.4%)
3	LD	0.46	0/1007	0.62	0/1371
3	LE	0.39	0/1007	0.54	0/1371
3	LF	0.28	0/1007	0.61	2/1371 (0.1%)
3	LG	0.42	0/1007	0.67	1/1371 (0.1%)
3	LH	0.28	0/1007	0.55	0/1371
3	LI	0.36	0/1007	0.60	3/1371 (0.2%)
3	LJ	0.30	0/1007	0.51	0/1371
3	LK	0.37	0/1007	0.60	1/1371 (0.1%)
3	LL	0.39	0/1007	0.62	2/1371 (0.1%)
3	LM	0.37	0/1007	0.55	1/1371 (0.1%)
3	LN	0.36	0/1007	0.54	0/1371
3	MA	0.46	0/1007	0.69	2/1371 (0.1%)
3	MB	0.42	0/1007	0.58	0/1371
3	MC	0.41	0/1007	0.58	1/1371 (0.1%)
3	MD	0.40	0/1007	0.61	2/1371 (0.1%)
3	ME	0.41	0/1007	0.52	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	MF	0.60	1/1007 (0.1%)	0.73	5/1371 (0.4%)
3	MG	0.44	0/1007	0.65	3/1371 (0.2%)
3	MH	0.38	0/1007	0.51	0/1371
3	MI	0.41	0/1007	0.57	0/1371
3	MJ	0.38	0/1007	0.65	3/1371 (0.2%)
3	MK	0.39	0/1007	0.55	0/1371
3	ML	0.38	0/1007	0.55	0/1371
3	MM	0.42	0/1007	0.69	5/1371 (0.4%)
3	MN	0.38	0/1007	0.55	0/1371
3	NA	0.39	0/1007	0.54	0/1371
3	NB	0.41	0/1007	0.63	2/1371 (0.1%)
3	NC	0.41	0/1007	0.65	1/1371 (0.1%)
3	ND	0.41	0/1007	0.52	0/1371
3	NE	0.45	0/1007	0.72	3/1371 (0.2%)
3	NF	0.43	0/1007	0.58	0/1371
3	NG	0.41	0/1007	0.53	0/1371
3	NH	0.40	0/1007	0.61	3/1371 (0.2%)
3	NI	0.40	0/1007	0.53	0/1371
3	NJ	0.55	2/1007 (0.2%)	0.75	4/1371 (0.3%)
All	All	0.34	8/284406 (0.0%)	0.51	204/406716 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	BB	0	1
3	BD	0	1
3	BG	0	1
3	BH	0	1
3	BM	0	1
3	BN	0	1
3	CC	0	1
3	CH	0	1
3	CI	0	1
3	CJ	0	1
3	CK	0	1
3	CN	0	1
3	DC	0	1
3	DF	0	1
3	DI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	DL	0	1
3	EB	0	1
3	EF	0	1
3	EI	0	1
3	EM	0	1
3	FC	0	1
3	FE	0	1
3	FG	0	1
3	FJ	0	1
3	FK	0	2
3	GD	0	1
3	GG	0	3
3	HA	0	1
3	HB	0	1
3	HE	0	1
3	HH	0	1
3	HK	0	1
3	HL	0	1
3	HN	0	1
3	IC	0	1
3	IE	0	1
3	IG	0	1
3	II	0	1
3	JA	0	1
3	JC	0	1
3	JF	0	1
3	JG	0	1
3	JK	0	1
3	JL	0	1
3	JM	0	1
3	JN	0	1
3	KB	0	1
3	KE	0	1
3	KH	0	2
3	KI	0	1
3	LI	0	1
3	LJ	0	1
3	LK	0	1
3	LL	0	1
3	MA	0	1
3	MB	0	1
3	ME	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	MF	0	1
3	MI	0	1
3	MK	0	1
3	ML	0	1
3	MM	0	1
3	NB	0	1
3	ND	0	1
3	NG	0	1
3	NH	0	1
3	NI	0	1
All	All	0	71

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	MF	21	LEU	C-N	-11.83	1.17	1.33
3	NJ	55	PRO	CG-CD	-10.44	1.15	1.50
3	LC	130	PRO	CG-CD	-8.88	1.20	1.50
3	DH	55	PRO	CG-CD	-7.45	1.25	1.50
3	HD	42	PRO	CG-CD	-6.09	1.30	1.50

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LC	130	PRO	N-CD-CG	-12.04	85.14	103.20
3	NJ	55	PRO	N-CD-CG	-11.92	85.32	103.20
3	HD	42	PRO	CA-N-CD	-11.00	96.60	112.00
3	DH	55	PRO	N-CD-CG	-10.86	86.91	103.20
3	NJ	55	PRO	CA-N-CD	-10.70	97.02	112.00

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	BB	79	SER	Peptide
3	BD	60	LYS	Peptide
3	BG	60	LYS	Peptide
3	BH	79	SER	Peptide
3	BM	60	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	89319	0	45162	3451	0
2	M	3438	0	3381	142	0
3	B	993	0	1008	42	0
3	BA	993	0	1006	115	0
3	BB	993	0	1006	129	0
3	BC	993	0	1006	114	0
3	BD	993	0	1006	126	0
3	BE	993	0	1006	101	0
3	BF	993	0	1006	102	0
3	BG	993	0	1006	100	0
3	BH	993	0	1006	103	0
3	BI	993	0	1006	124	0
3	BJ	993	0	1006	108	0
3	BK	993	0	1006	119	0
3	BL	993	0	1006	103	0
3	BM	993	0	1006	93	0
3	BN	993	0	1006	112	0
3	CA	993	0	1006	105	0
3	CB	993	0	1006	141	0
3	CC	993	0	1006	122	0
3	CD	993	0	1006	101	0
3	CE	993	0	1006	107	0
3	CF	993	0	1006	114	0
3	CG	993	0	1006	103	0
3	CH	993	0	1006	114	0
3	CI	993	0	1006	114	0
3	CJ	993	0	1006	112	0
3	CK	993	0	1006	107	0
3	CL	993	0	1006	95	0
3	CM	993	0	1006	113	0
3	CN	993	0	1006	117	0
3	D	993	0	1008	38	0
3	DA	993	0	1006	107	0
3	DB	993	0	1006	122	0
3	DC	993	0	1006	111	0
3	DD	993	0	1006	117	0
3	DE	993	0	1006	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DF	993	0	1006	135	0
3	DG	993	0	1006	137	0
3	DH	993	0	1006	105	0
3	DI	993	0	1006	105	0
3	DJ	993	0	1006	107	0
3	DK	993	0	1006	113	0
3	DL	993	0	1006	114	0
3	DM	993	0	1006	103	0
3	DN	993	0	1006	87	0
3	EA	993	0	1006	98	0
3	EB	993	0	1006	126	0
3	EC	993	0	1006	118	0
3	ED	993	0	1006	116	0
3	EE	993	0	1006	127	0
3	EF	993	0	1006	98	0
3	EG	993	0	1007	110	0
3	EH	993	0	1006	99	0
3	EI	993	0	1006	138	0
3	EJ	993	0	1006	163	0
3	EK	993	0	1006	107	0
3	EL	993	0	1006	135	0
3	EM	993	0	1006	96	0
3	EN	993	0	1006	101	0
3	FA	993	0	1006	106	0
3	FB	993	0	1006	106	0
3	FC	993	0	1006	83	0
3	FD	930	0	955	63	0
3	FE	993	0	1006	111	0
3	FF	993	0	1006	97	0
3	FG	993	0	1006	80	0
3	FH	993	0	1007	124	0
3	FI	993	0	1006	124	0
3	FJ	993	0	1006	136	0
3	FK	993	0	1006	132	0
3	FL	993	0	1006	93	0
3	FM	993	0	1006	115	0
3	FN	993	0	1006	116	0
3	GA	993	0	1006	122	0
3	GB	942	0	965	67	0
3	GC	993	0	1006	109	0
3	GD	993	0	1006	137	0
3	GE	993	0	1006	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GF	993	0	1006	106	0
3	GG	993	0	1006	137	0
3	GH	993	0	1006	131	0
3	GI	993	0	1006	96	0
3	GJ	993	0	1006	136	0
3	GK	993	0	1006	124	0
3	GL	993	0	1006	119	0
3	GM	993	0	1006	133	0
3	GN	993	0	1006	122	0
3	HA	993	0	1006	95	0
3	HB	993	0	1006	115	0
3	HC	993	0	1006	123	0
3	HD	993	0	1006	104	0
3	HE	993	0	1006	110	0
3	HF	993	0	1006	113	0
3	HG	993	0	1006	104	0
3	HH	993	0	1006	109	0
3	HI	993	0	1006	118	0
3	HJ	993	0	1006	131	0
3	HK	993	0	1006	108	0
3	HL	993	0	1006	114	0
3	HM	993	0	1006	111	0
3	HN	993	0	1006	106	0
3	IA	993	0	1006	112	0
3	IB	993	0	1006	102	0
3	IC	993	0	1006	106	0
3	ID	993	0	1006	128	0
3	IE	993	0	1006	128	0
3	IF	993	0	1006	98	0
3	IG	993	0	1006	112	0
3	IH	993	0	1006	114	0
3	II	993	0	1006	133	0
3	IJ	993	0	1006	118	0
3	IK	993	0	1006	100	0
3	IL	993	0	1006	123	0
3	IM	993	0	1006	82	0
3	IN	993	0	1006	91	0
3	JA	993	0	1006	138	0
3	JB	993	0	1006	120	0
3	JC	993	0	1006	105	0
3	JD	993	0	1006	104	0
3	JE	993	0	1006	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	JF	993	0	1006	96	0
3	JG	993	0	1006	113	0
3	JH	993	0	1006	93	0
3	JI	993	0	1006	102	0
3	JJ	993	0	1006	123	0
3	JK	993	0	1006	116	0
3	JL	993	0	1006	96	0
3	JM	993	0	1006	103	0
3	JN	993	0	1006	102	0
3	KA	993	0	1006	95	0
3	KB	993	0	1006	120	0
3	KC	993	0	1006	120	0
3	KD	993	0	1006	78	0
3	KE	993	0	1007	118	0
3	KF	993	0	1006	123	0
3	KG	993	0	1006	90	0
3	KH	993	0	1006	136	0
3	KI	993	0	1006	112	0
3	KJ	993	0	1006	121	0
3	KK	993	0	1006	136	0
3	KL	993	0	1006	108	0
3	KM	993	0	1006	117	0
3	KN	993	0	1006	130	0
3	LA	993	0	1006	117	0
3	LB	993	0	1006	99	0
3	LC	993	0	1006	101	0
3	LD	993	0	1006	114	0
3	LE	993	0	1006	119	0
3	LF	993	0	1007	86	0
3	LG	993	0	1006	136	0
3	LH	993	0	1006	93	0
3	LI	993	0	1006	84	0
3	LJ	993	0	1006	96	0
3	LK	993	0	1006	107	0
3	LL	993	0	1006	116	0
3	LM	993	0	1006	104	0
3	LN	993	0	1006	118	0
3	MA	993	0	1006	147	0
3	MB	993	0	1006	120	0
3	MC	993	0	1006	118	0
3	MD	993	0	1006	113	0
3	ME	993	0	1006	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	MF	993	0	1006	125	0
3	MG	993	0	1006	130	0
3	MH	993	0	1006	119	0
3	MI	993	0	1006	141	0
3	MJ	993	0	1006	117	0
3	MK	993	0	1006	111	0
3	ML	993	0	1006	104	0
3	MM	993	0	1006	130	0
3	MN	993	0	1006	120	0
3	NA	993	0	1006	110	0
3	NB	993	0	1006	114	0
3	NC	993	0	1006	114	0
3	ND	993	0	1006	113	0
3	NE	993	0	1006	118	0
3	NF	993	0	1006	100	0
3	NG	993	0	1006	100	0
3	NH	993	0	1006	114	0
3	NI	993	0	1006	102	0
3	NJ	993	0	1006	138	0
All	All	271383	0	229539	17336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 17336 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BF:8:LEU:HD11	3:IN:114:ALA:HB1	1.24	1.14
3:DM:103:GLU:OE2	3:EM:13:LYS:NZ	1.82	1.13
3:BI:8:LEU:HD12	3:HM:114:ALA:HB1	1.25	1.11
3:GG:86:ARG:NH2	3:JE:99:TYR:O	1.83	1.11
3:JM:82:PRO:O	3:KA:99:TYR:OH	1.66	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	417/420 (99%)	381 (91%)	36 (9%)	0	100	100
3	B	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	BA	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	BB	130/133 (98%)	114 (88%)	14 (11%)	2 (2%)	8	38
3	BC	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	BD	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	BE	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	BF	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	BG	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	BH	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	BI	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	BJ	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	BK	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	BL	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	BM	130/133 (98%)	108 (83%)	22 (17%)	0	100	100
3	BN	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	CA	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	CB	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	CC	130/133 (98%)	112 (86%)	17 (13%)	1 (1%)	16	53
3	CD	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	CE	130/133 (98%)	109 (84%)	21 (16%)	0	100	100
3	CF	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	CG	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	CH	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	CI	130/133 (98%)	112 (86%)	17 (13%)	1 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CJ	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	CK	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	CL	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	CM	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	CN	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	D	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	DA	130/133 (98%)	111 (85%)	18 (14%)	1 (1%)	16	53
3	DB	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	DC	130/133 (98%)	108 (83%)	22 (17%)	0	100	100
3	DD	130/133 (98%)	111 (85%)	18 (14%)	1 (1%)	16	53
3	DE	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	DF	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	DG	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	DH	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	DI	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	DJ	130/133 (98%)	108 (83%)	21 (16%)	1 (1%)	16	53
3	DK	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	DL	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	DM	130/133 (98%)	110 (85%)	19 (15%)	1 (1%)	16	53
3	DN	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	EA	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	EB	130/133 (98%)	108 (83%)	21 (16%)	1 (1%)	16	53
3	EC	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	ED	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	EE	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	EF	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	EG	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	EH	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	EI	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	EJ	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	EK	130/133 (98%)	111 (85%)	18 (14%)	1 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EL	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	EM	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	EN	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	FA	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	FB	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	FC	130/133 (98%)	115 (88%)	14 (11%)	1 (1%)	16	53
3	FD	118/133 (89%)	108 (92%)	10 (8%)	0	100	100
3	FE	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	FF	130/133 (98%)	118 (91%)	11 (8%)	1 (1%)	16	53
3	FG	130/133 (98%)	119 (92%)	11 (8%)	0	100	100
3	FH	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	FI	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	FJ	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	FK	130/133 (98%)	119 (92%)	10 (8%)	1 (1%)	16	53
3	FL	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	FM	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	FN	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	GA	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	GB	120/133 (90%)	107 (89%)	13 (11%)	0	100	100
3	GC	130/133 (98%)	108 (83%)	22 (17%)	0	100	100
3	GD	130/133 (98%)	109 (84%)	21 (16%)	0	100	100
3	GE	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	GF	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	GG	130/133 (98%)	109 (84%)	21 (16%)	0	100	100
3	GH	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	GI	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	GJ	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	GK	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	GL	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	GM	130/133 (98%)	109 (84%)	20 (15%)	1 (1%)	16	53
3	GN	130/133 (98%)	109 (84%)	21 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	HA	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	HB	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	HC	130/133 (98%)	115 (88%)	14 (11%)	1 (1%)	16	53
3	HD	130/133 (98%)	119 (92%)	11 (8%)	0	100	100
3	HE	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	HF	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	HG	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	HH	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	HI	130/133 (98%)	113 (87%)	16 (12%)	1 (1%)	16	53
3	HJ	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	HK	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	HL	130/133 (98%)	111 (85%)	18 (14%)	1 (1%)	16	53
3	HM	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	HN	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	IA	130/133 (98%)	112 (86%)	16 (12%)	2 (2%)	8	38
3	IB	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	IC	130/133 (98%)	109 (84%)	21 (16%)	0	100	100
3	ID	130/133 (98%)	112 (86%)	17 (13%)	1 (1%)	16	53
3	IE	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	IF	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	IG	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	IH	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	II	130/133 (98%)	110 (85%)	20 (15%)	0	100	100
3	IJ	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	IK	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	IL	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	IM	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	IN	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	JA	130/133 (98%)	109 (84%)	21 (16%)	0	100	100
3	JB	130/133 (98%)	116 (89%)	13 (10%)	1 (1%)	16	53
3	JC	130/133 (98%)	116 (89%)	14 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	JD	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	JE	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	JF	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	JG	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	JH	130/133 (98%)	109 (84%)	20 (15%)	1 (1%)	16	53
3	JI	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	JJ	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	JK	130/133 (98%)	112 (86%)	17 (13%)	1 (1%)	16	53
3	JL	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	JM	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	JN	130/133 (98%)	113 (87%)	16 (12%)	1 (1%)	16	53
3	KA	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	KB	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	KC	130/133 (98%)	113 (87%)	16 (12%)	1 (1%)	16	53
3	KD	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	KE	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	KF	130/133 (98%)	105 (81%)	24 (18%)	1 (1%)	16	53
3	KG	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	KH	130/133 (98%)	110 (85%)	19 (15%)	1 (1%)	16	53
3	KI	130/133 (98%)	115 (88%)	14 (11%)	1 (1%)	16	53
3	KJ	130/133 (98%)	117 (90%)	12 (9%)	1 (1%)	16	53
3	KK	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	KL	130/133 (98%)	116 (89%)	13 (10%)	1 (1%)	16	53
3	KM	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	KN	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	LA	130/133 (98%)	114 (88%)	15 (12%)	1 (1%)	16	53
3	LB	130/133 (98%)	119 (92%)	11 (8%)	0	100	100
3	LC	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	LD	130/133 (98%)	115 (88%)	14 (11%)	1 (1%)	16	53
3	LE	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	LF	130/133 (98%)	117 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LG	130/133 (98%)	113 (87%)	16 (12%)	1 (1%)	16	53
3	LH	130/133 (98%)	120 (92%)	10 (8%)	0	100	100
3	LI	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	LJ	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	LK	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	LL	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	LM	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	LN	130/133 (98%)	117 (90%)	13 (10%)	0	100	100
3	MA	130/133 (98%)	115 (88%)	15 (12%)	0	100	100
3	MB	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	MC	130/133 (98%)	120 (92%)	9 (7%)	1 (1%)	16	53
3	MD	130/133 (98%)	111 (85%)	19 (15%)	0	100	100
3	ME	130/133 (98%)	112 (86%)	17 (13%)	1 (1%)	16	53
3	MF	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	MG	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	MH	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	MI	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	MJ	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	MK	130/133 (98%)	116 (89%)	13 (10%)	1 (1%)	16	53
3	ML	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	MM	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	MN	130/133 (98%)	109 (84%)	20 (15%)	1 (1%)	16	53
3	NA	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	NB	130/133 (98%)	109 (84%)	21 (16%)	0	100	100
3	NC	130/133 (98%)	112 (86%)	17 (13%)	1 (1%)	16	53
3	ND	130/133 (98%)	114 (88%)	16 (12%)	0	100	100
3	NE	130/133 (98%)	112 (86%)	18 (14%)	0	100	100
3	NF	130/133 (98%)	113 (87%)	17 (13%)	0	100	100
3	NG	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
3	NH	130/133 (98%)	116 (89%)	14 (11%)	0	100	100
3	NI	130/133 (98%)	118 (91%)	11 (8%)	1 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	NJ	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
All	All	23795/24360 (98%)	20848 (88%)	2902 (12%)	45 (0%)	44	77

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	BB	80	CYS
3	BH	80	CYS
3	CI	80	CYS
3	DE	61	ASN
3	FK	80	CYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	365/366 (100%)	365 (100%)	0	100	100
3	B	110/111 (99%)	110 (100%)	0	100	100
3	BA	110/111 (99%)	110 (100%)	0	100	100
3	BB	110/111 (99%)	110 (100%)	0	100	100
3	BC	110/111 (99%)	110 (100%)	0	100	100
3	BD	110/111 (99%)	110 (100%)	0	100	100
3	BE	110/111 (99%)	110 (100%)	0	100	100
3	BF	110/111 (99%)	110 (100%)	0	100	100
3	BG	110/111 (99%)	110 (100%)	0	100	100
3	BH	110/111 (99%)	110 (100%)	0	100	100
3	BI	110/111 (99%)	110 (100%)	0	100	100
3	BJ	110/111 (99%)	110 (100%)	0	100	100
3	BK	110/111 (99%)	110 (100%)	0	100	100
3	BL	110/111 (99%)	110 (100%)	0	100	100
3	BM	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BN	110/111 (99%)	110 (100%)	0	100	100
3	CA	110/111 (99%)	110 (100%)	0	100	100
3	CB	110/111 (99%)	110 (100%)	0	100	100
3	CC	110/111 (99%)	110 (100%)	0	100	100
3	CD	110/111 (99%)	110 (100%)	0	100	100
3	CE	110/111 (99%)	110 (100%)	0	100	100
3	CF	110/111 (99%)	110 (100%)	0	100	100
3	CG	110/111 (99%)	110 (100%)	0	100	100
3	CH	110/111 (99%)	110 (100%)	0	100	100
3	CI	110/111 (99%)	110 (100%)	0	100	100
3	CJ	110/111 (99%)	110 (100%)	0	100	100
3	CK	110/111 (99%)	110 (100%)	0	100	100
3	CL	110/111 (99%)	110 (100%)	0	100	100
3	CM	110/111 (99%)	110 (100%)	0	100	100
3	CN	110/111 (99%)	110 (100%)	0	100	100
3	D	110/111 (99%)	110 (100%)	0	100	100
3	DA	110/111 (99%)	110 (100%)	0	100	100
3	DB	110/111 (99%)	110 (100%)	0	100	100
3	DC	110/111 (99%)	110 (100%)	0	100	100
3	DD	110/111 (99%)	110 (100%)	0	100	100
3	DE	110/111 (99%)	110 (100%)	0	100	100
3	DF	110/111 (99%)	110 (100%)	0	100	100
3	DG	110/111 (99%)	110 (100%)	0	100	100
3	DH	110/111 (99%)	110 (100%)	0	100	100
3	DI	110/111 (99%)	110 (100%)	0	100	100
3	DJ	110/111 (99%)	110 (100%)	0	100	100
3	DK	110/111 (99%)	110 (100%)	0	100	100
3	DL	110/111 (99%)	110 (100%)	0	100	100
3	DM	110/111 (99%)	110 (100%)	0	100	100
3	DN	110/111 (99%)	110 (100%)	0	100	100
3	EA	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	EB	110/111 (99%)	110 (100%)	0	100	100
3	EC	110/111 (99%)	110 (100%)	0	100	100
3	ED	110/111 (99%)	110 (100%)	0	100	100
3	EE	110/111 (99%)	110 (100%)	0	100	100
3	EF	110/111 (99%)	110 (100%)	0	100	100
3	EG	110/111 (99%)	110 (100%)	0	100	100
3	EH	110/111 (99%)	110 (100%)	0	100	100
3	EI	110/111 (99%)	110 (100%)	0	100	100
3	EJ	110/111 (99%)	109 (99%)	1 (1%)	70	76
3	EK	110/111 (99%)	110 (100%)	0	100	100
3	EL	110/111 (99%)	110 (100%)	0	100	100
3	EM	110/111 (99%)	110 (100%)	0	100	100
3	EN	110/111 (99%)	110 (100%)	0	100	100
3	FA	110/111 (99%)	110 (100%)	0	100	100
3	FB	110/111 (99%)	110 (100%)	0	100	100
3	FC	110/111 (99%)	110 (100%)	0	100	100
3	FD	102/111 (92%)	102 (100%)	0	100	100
3	FE	110/111 (99%)	110 (100%)	0	100	100
3	FF	110/111 (99%)	110 (100%)	0	100	100
3	FG	110/111 (99%)	110 (100%)	0	100	100
3	FH	110/111 (99%)	110 (100%)	0	100	100
3	FI	110/111 (99%)	110 (100%)	0	100	100
3	FJ	110/111 (99%)	110 (100%)	0	100	100
3	FK	110/111 (99%)	110 (100%)	0	100	100
3	FL	110/111 (99%)	110 (100%)	0	100	100
3	FM	110/111 (99%)	110 (100%)	0	100	100
3	FN	110/111 (99%)	110 (100%)	0	100	100
3	GA	110/111 (99%)	110 (100%)	0	100	100
3	GB	104/111 (94%)	104 (100%)	0	100	100
3	GC	110/111 (99%)	110 (100%)	0	100	100
3	GD	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	GE	110/111 (99%)	110 (100%)	0	100	100
3	GF	110/111 (99%)	110 (100%)	0	100	100
3	GG	110/111 (99%)	110 (100%)	0	100	100
3	GH	110/111 (99%)	110 (100%)	0	100	100
3	GI	110/111 (99%)	110 (100%)	0	100	100
3	GJ	110/111 (99%)	110 (100%)	0	100	100
3	GK	110/111 (99%)	110 (100%)	0	100	100
3	GL	110/111 (99%)	110 (100%)	0	100	100
3	GM	110/111 (99%)	110 (100%)	0	100	100
3	GN	110/111 (99%)	110 (100%)	0	100	100
3	HA	110/111 (99%)	110 (100%)	0	100	100
3	HB	110/111 (99%)	110 (100%)	0	100	100
3	HC	110/111 (99%)	110 (100%)	0	100	100
3	HD	110/111 (99%)	110 (100%)	0	100	100
3	HE	110/111 (99%)	110 (100%)	0	100	100
3	HF	110/111 (99%)	110 (100%)	0	100	100
3	HG	110/111 (99%)	110 (100%)	0	100	100
3	HH	110/111 (99%)	110 (100%)	0	100	100
3	HI	110/111 (99%)	110 (100%)	0	100	100
3	HJ	110/111 (99%)	110 (100%)	0	100	100
3	HK	110/111 (99%)	110 (100%)	0	100	100
3	HL	110/111 (99%)	110 (100%)	0	100	100
3	HM	110/111 (99%)	110 (100%)	0	100	100
3	HN	110/111 (99%)	110 (100%)	0	100	100
3	IA	110/111 (99%)	110 (100%)	0	100	100
3	IB	110/111 (99%)	110 (100%)	0	100	100
3	IC	110/111 (99%)	110 (100%)	0	100	100
3	ID	110/111 (99%)	110 (100%)	0	100	100
3	IE	110/111 (99%)	110 (100%)	0	100	100
3	IF	110/111 (99%)	110 (100%)	0	100	100
3	IG	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	IH	110/111 (99%)	110 (100%)	0	100	100
3	II	110/111 (99%)	110 (100%)	0	100	100
3	IJ	110/111 (99%)	110 (100%)	0	100	100
3	IK	110/111 (99%)	110 (100%)	0	100	100
3	IL	110/111 (99%)	110 (100%)	0	100	100
3	IM	110/111 (99%)	110 (100%)	0	100	100
3	IN	110/111 (99%)	110 (100%)	0	100	100
3	JA	110/111 (99%)	110 (100%)	0	100	100
3	JB	110/111 (99%)	110 (100%)	0	100	100
3	JC	110/111 (99%)	110 (100%)	0	100	100
3	JD	110/111 (99%)	110 (100%)	0	100	100
3	JE	110/111 (99%)	110 (100%)	0	100	100
3	JF	110/111 (99%)	110 (100%)	0	100	100
3	JG	110/111 (99%)	110 (100%)	0	100	100
3	JH	110/111 (99%)	110 (100%)	0	100	100
3	JI	110/111 (99%)	110 (100%)	0	100	100
3	JJ	110/111 (99%)	110 (100%)	0	100	100
3	JK	110/111 (99%)	110 (100%)	0	100	100
3	JL	110/111 (99%)	110 (100%)	0	100	100
3	JM	110/111 (99%)	110 (100%)	0	100	100
3	JN	110/111 (99%)	110 (100%)	0	100	100
3	KA	110/111 (99%)	110 (100%)	0	100	100
3	KB	110/111 (99%)	110 (100%)	0	100	100
3	KC	110/111 (99%)	110 (100%)	0	100	100
3	KD	110/111 (99%)	110 (100%)	0	100	100
3	KE	110/111 (99%)	110 (100%)	0	100	100
3	KF	110/111 (99%)	110 (100%)	0	100	100
3	KG	110/111 (99%)	110 (100%)	0	100	100
3	KH	110/111 (99%)	110 (100%)	0	100	100
3	KI	110/111 (99%)	110 (100%)	0	100	100
3	KJ	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	KK	110/111 (99%)	110 (100%)	0	100	100
3	KL	110/111 (99%)	110 (100%)	0	100	100
3	KM	110/111 (99%)	110 (100%)	0	100	100
3	KN	110/111 (99%)	110 (100%)	0	100	100
3	LA	110/111 (99%)	110 (100%)	0	100	100
3	LB	110/111 (99%)	110 (100%)	0	100	100
3	LC	110/111 (99%)	110 (100%)	0	100	100
3	LD	110/111 (99%)	110 (100%)	0	100	100
3	LE	110/111 (99%)	110 (100%)	0	100	100
3	LF	110/111 (99%)	110 (100%)	0	100	100
3	LG	110/111 (99%)	110 (100%)	0	100	100
3	LH	110/111 (99%)	110 (100%)	0	100	100
3	LI	110/111 (99%)	110 (100%)	0	100	100
3	LJ	110/111 (99%)	110 (100%)	0	100	100
3	LK	110/111 (99%)	110 (100%)	0	100	100
3	LL	110/111 (99%)	110 (100%)	0	100	100
3	LM	110/111 (99%)	110 (100%)	0	100	100
3	LN	110/111 (99%)	110 (100%)	0	100	100
3	MA	110/111 (99%)	110 (100%)	0	100	100
3	MB	110/111 (99%)	110 (100%)	0	100	100
3	MC	110/111 (99%)	110 (100%)	0	100	100
3	MD	110/111 (99%)	110 (100%)	0	100	100
3	ME	110/111 (99%)	110 (100%)	0	100	100
3	MF	110/111 (99%)	110 (100%)	0	100	100
3	MG	110/111 (99%)	110 (100%)	0	100	100
3	MH	110/111 (99%)	110 (100%)	0	100	100
3	MI	110/111 (99%)	110 (100%)	0	100	100
3	MJ	110/111 (99%)	109 (99%)	1 (1%)	70	76
3	MK	110/111 (99%)	110 (100%)	0	100	100
3	ML	110/111 (99%)	110 (100%)	0	100	100
3	MM	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	MN	110/111 (99%)	110 (100%)	0	100	100
3	NA	110/111 (99%)	110 (100%)	0	100	100
3	NB	110/111 (99%)	110 (100%)	0	100	100
3	NC	110/111 (99%)	110 (100%)	0	100	100
3	ND	110/111 (99%)	110 (100%)	0	100	100
3	NE	110/111 (99%)	110 (100%)	0	100	100
3	NF	110/111 (99%)	110 (100%)	0	100	100
3	NG	110/111 (99%)	110 (100%)	0	100	100
3	NH	110/111 (99%)	110 (100%)	0	100	100
3	NI	110/111 (99%)	110 (100%)	0	100	100
3	NJ	110/111 (99%)	110 (100%)	0	100	100
All	All	20151/20346 (99%)	20149 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	EJ	58	ASN
3	MJ	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 224 such sidechains are listed below:

Mol	Chain	Res	Type
3	HH	127	GLN
3	NI	129	ASN
3	JG	22	ASN
3	NI	61	ASN
3	MK	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	4216/4217 (99%)	868 (20%)	83 (1%)

5 of 868 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	G
1	A	10	C
1	A	11	U
1	A	12	U
1	A	29	A

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3011	U
1	A	3798	A
1	A	3169	U
1	A	3555	U
1	A	3934	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	MF	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	MF	21:LEU	C	22:ASN	N	1.17

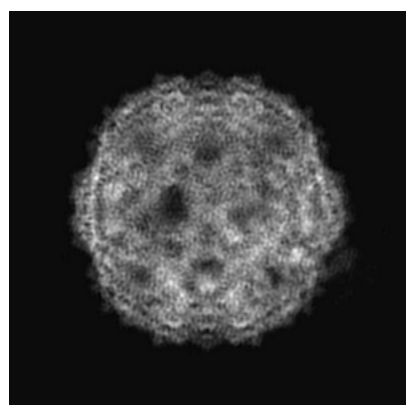
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23336. These allow visual inspection of the internal detail of the map and identification of artifacts.

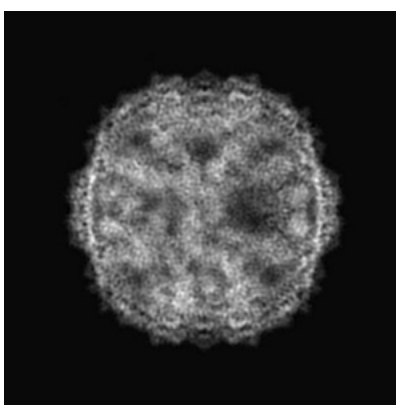
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

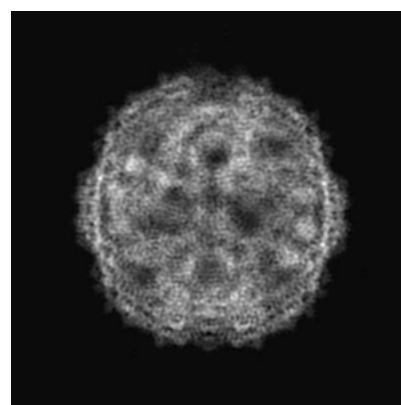
6.1.1 Primary map



X



Y

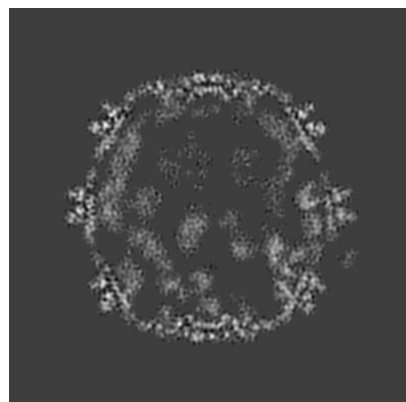


Z

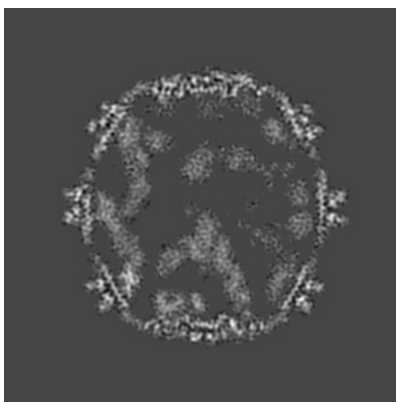
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

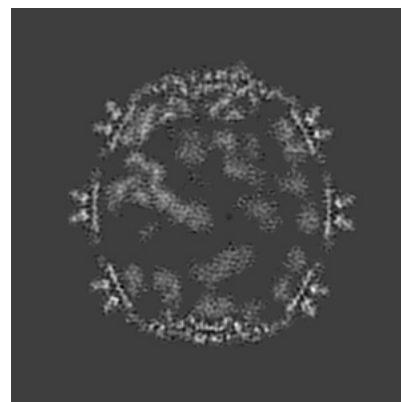
6.2.1 Primary map



X Index: 160



Y Index: 160

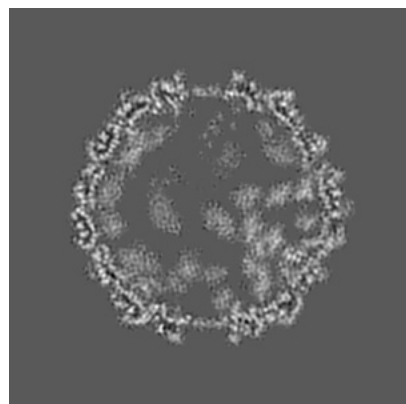


Z Index: 160

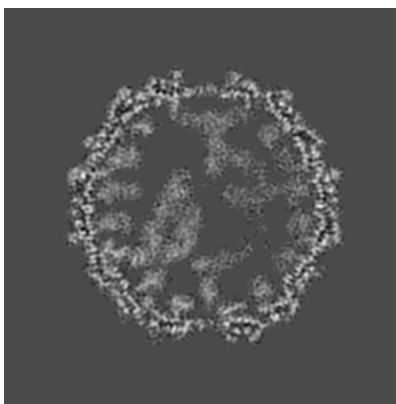
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

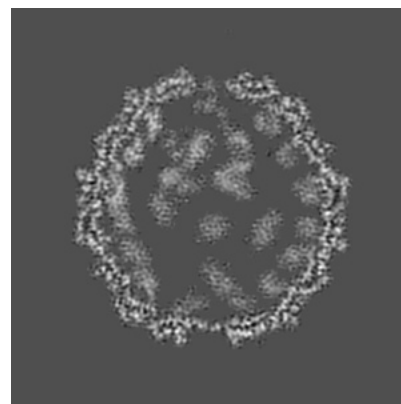
6.3.1 Primary map



X Index: 187



Y Index: 181

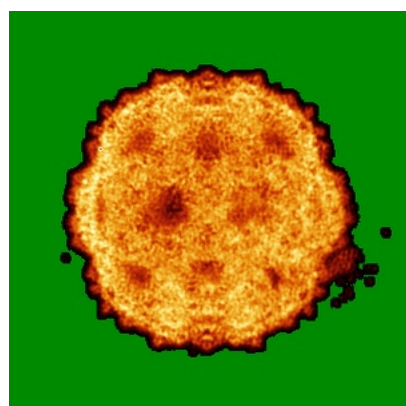


Z Index: 138

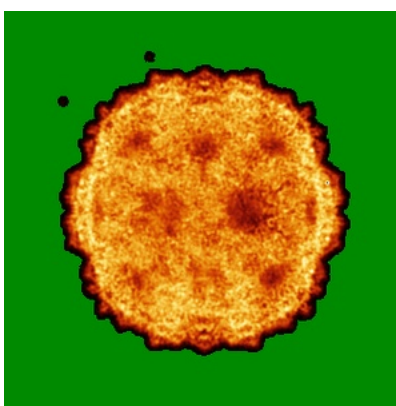
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

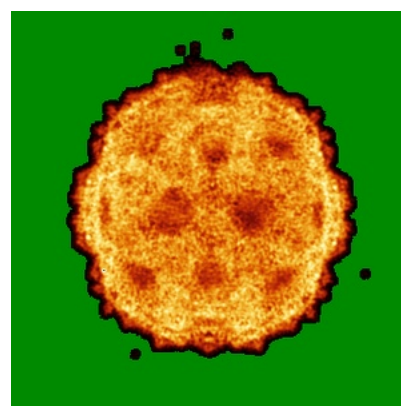
6.4.1 Primary map



X



Y

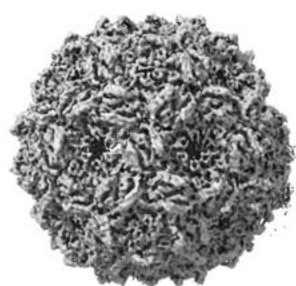


Z

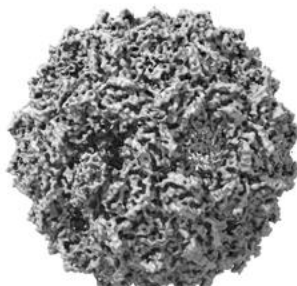
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

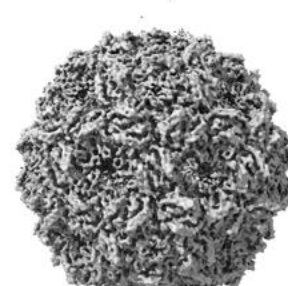
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

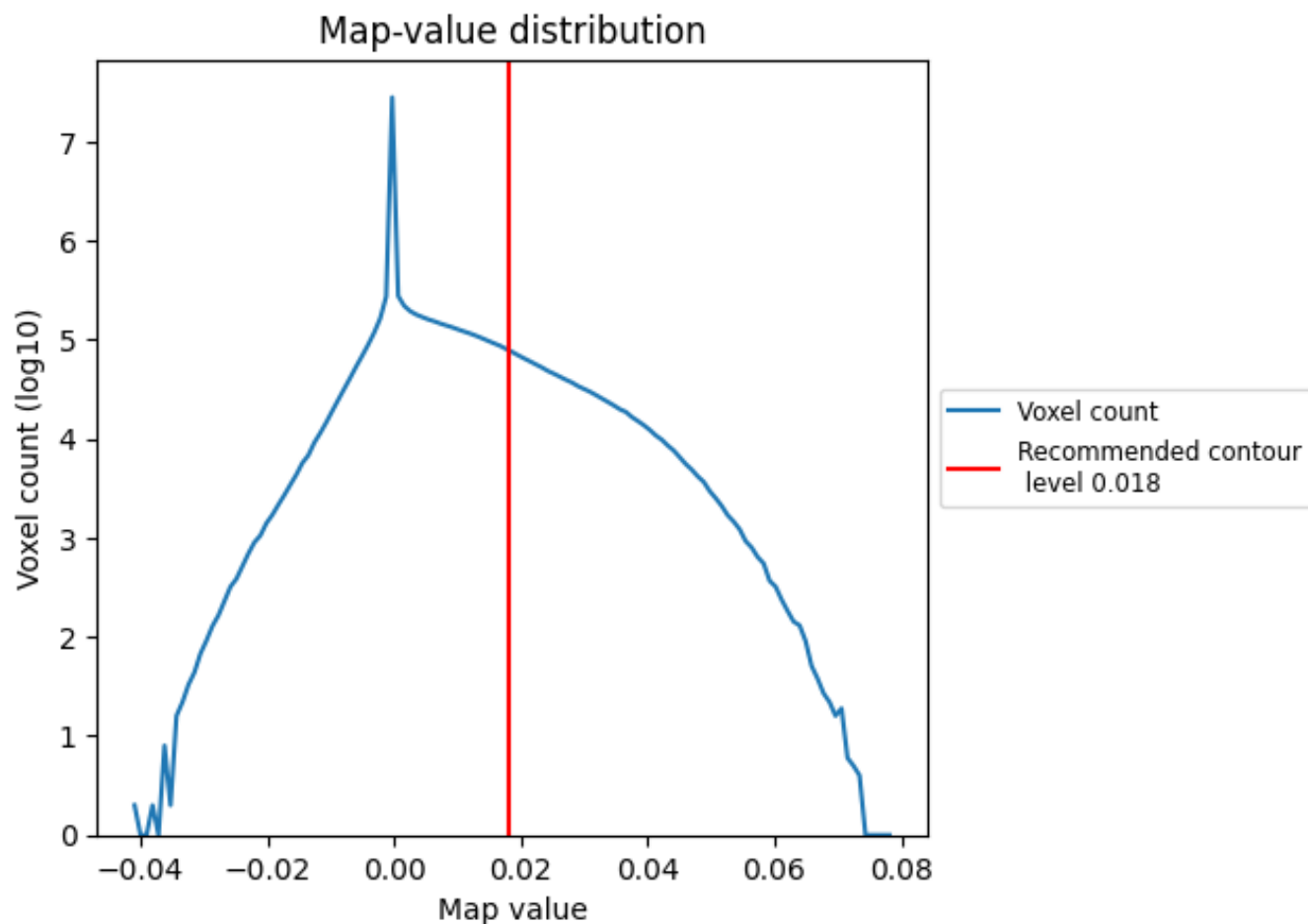
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

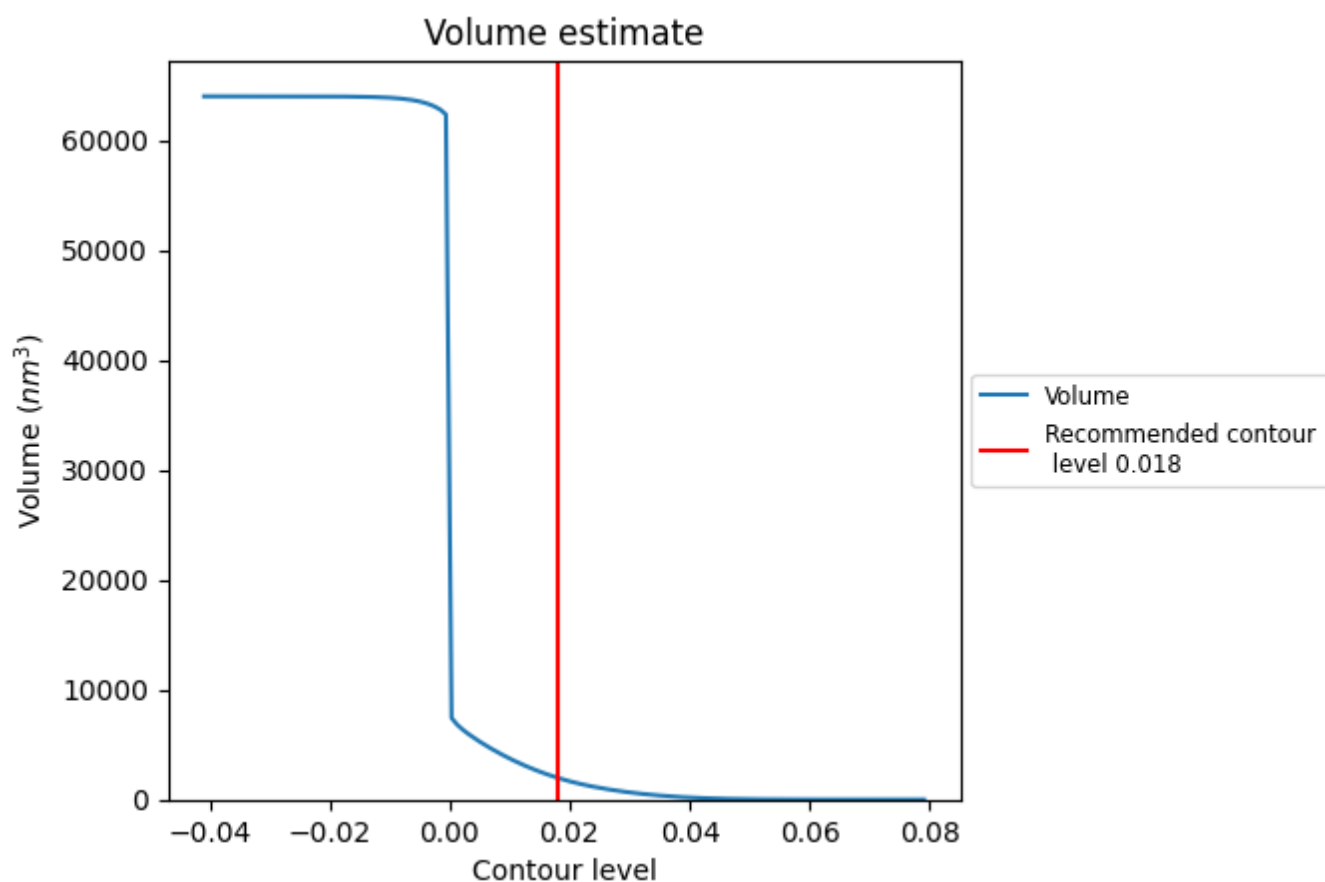
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

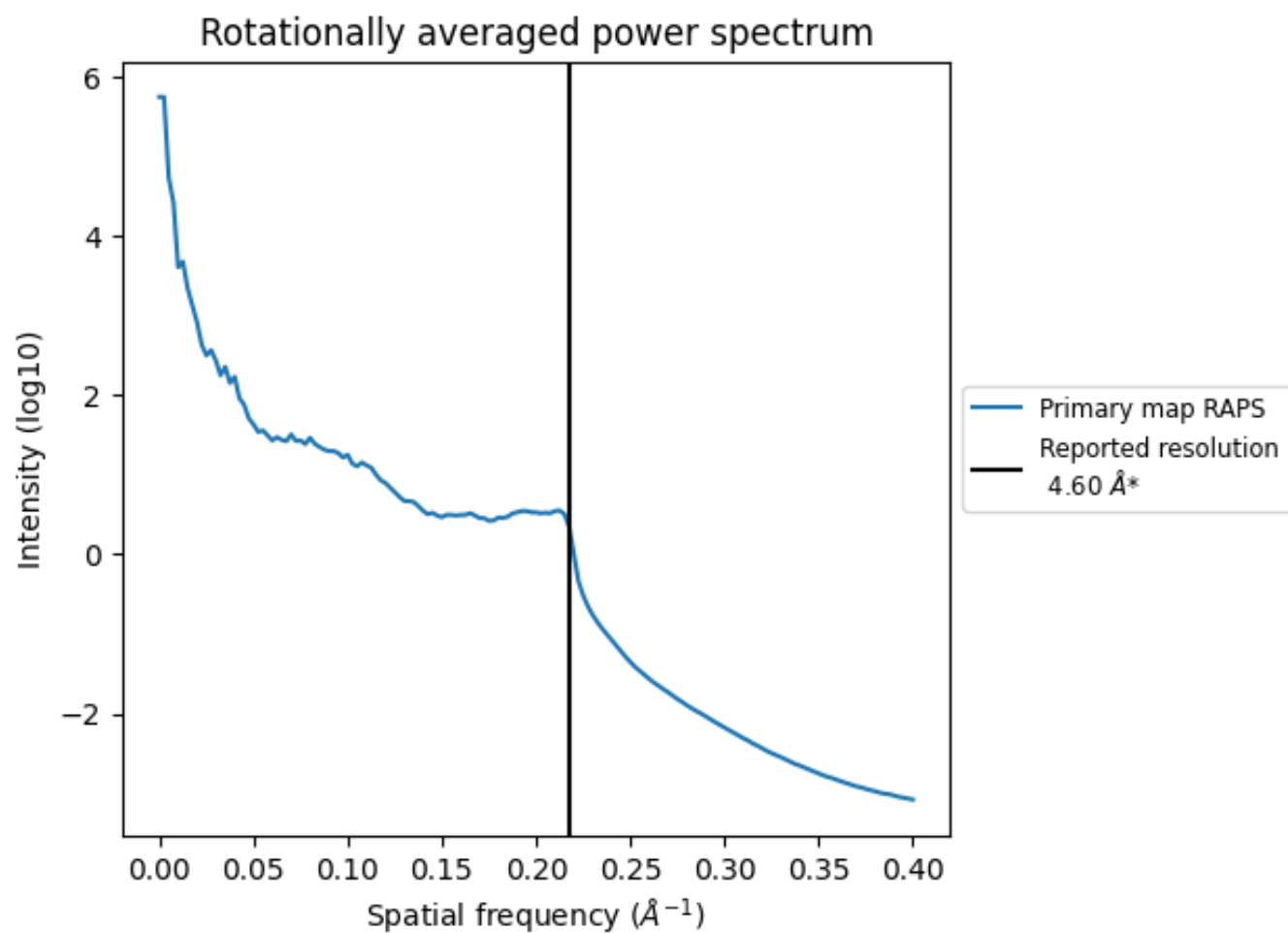
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1981 nm³; this corresponds to an approximate mass of 1790 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

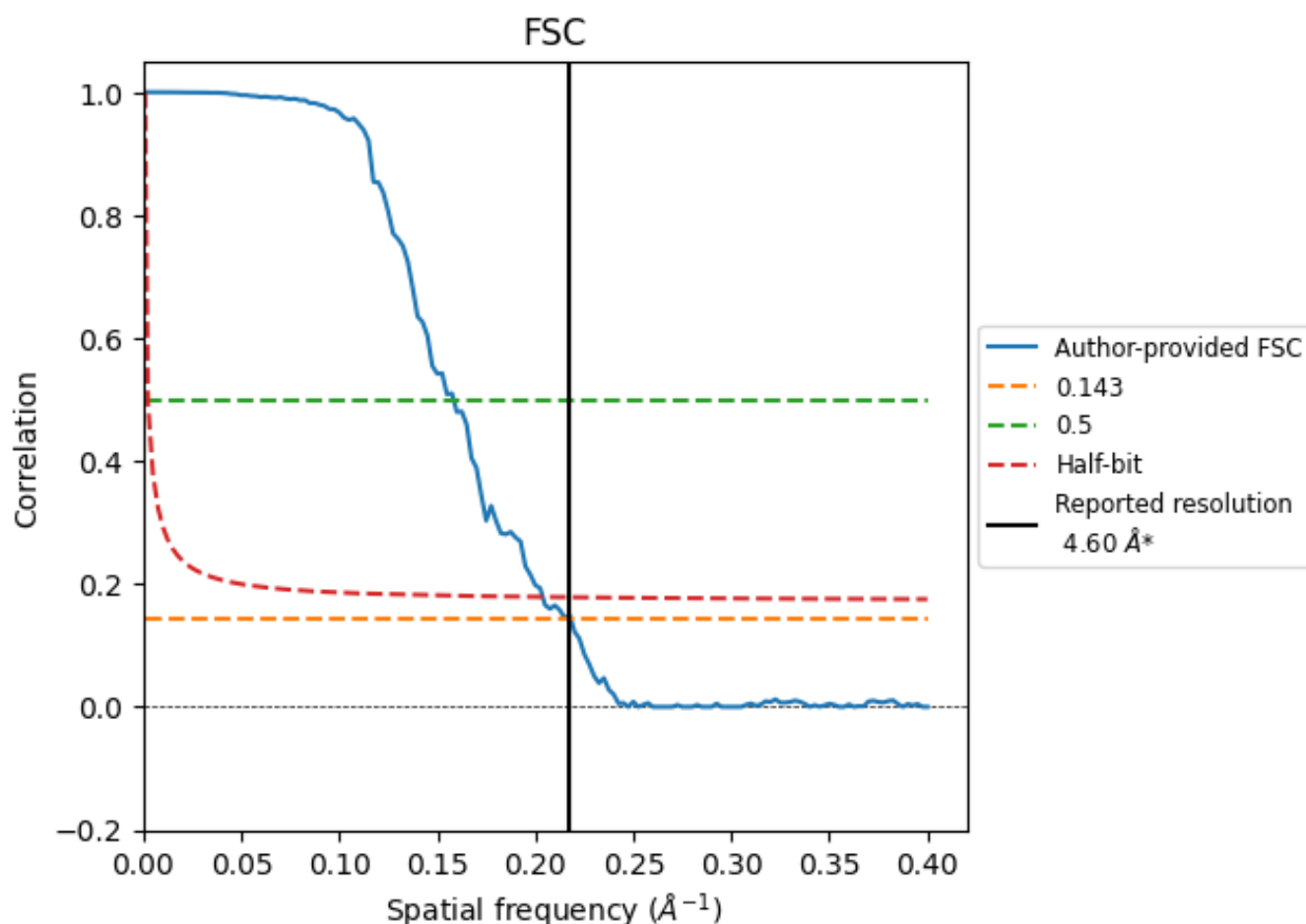


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

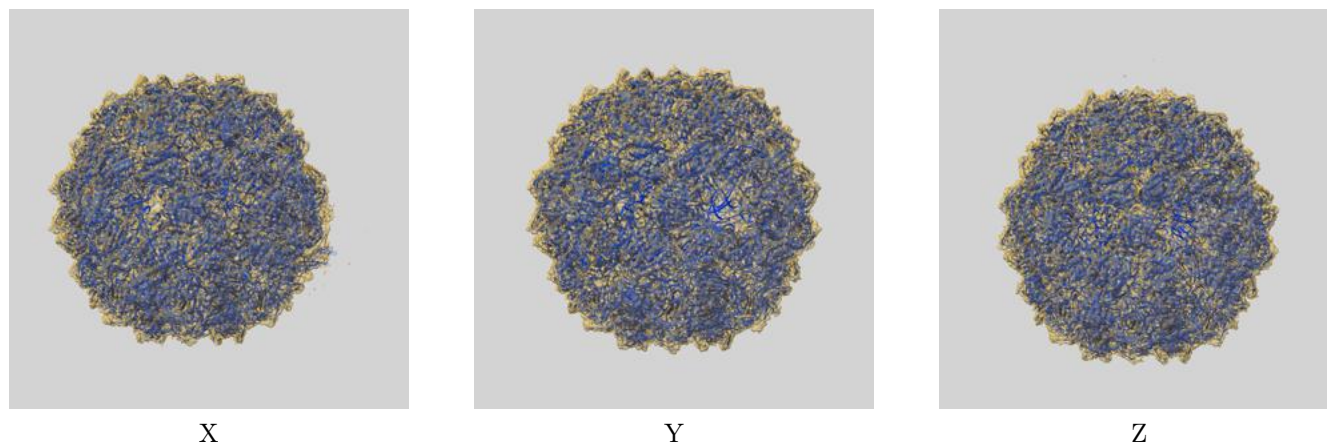
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.59	6.32	4.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

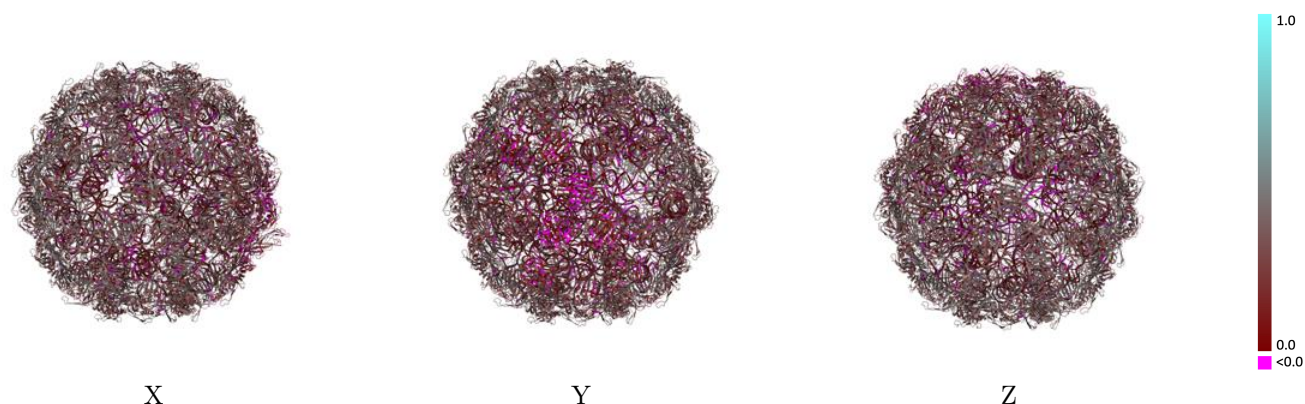
This section contains information regarding the fit between EMDB map EMD-23336 and PDB model 7LHD. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



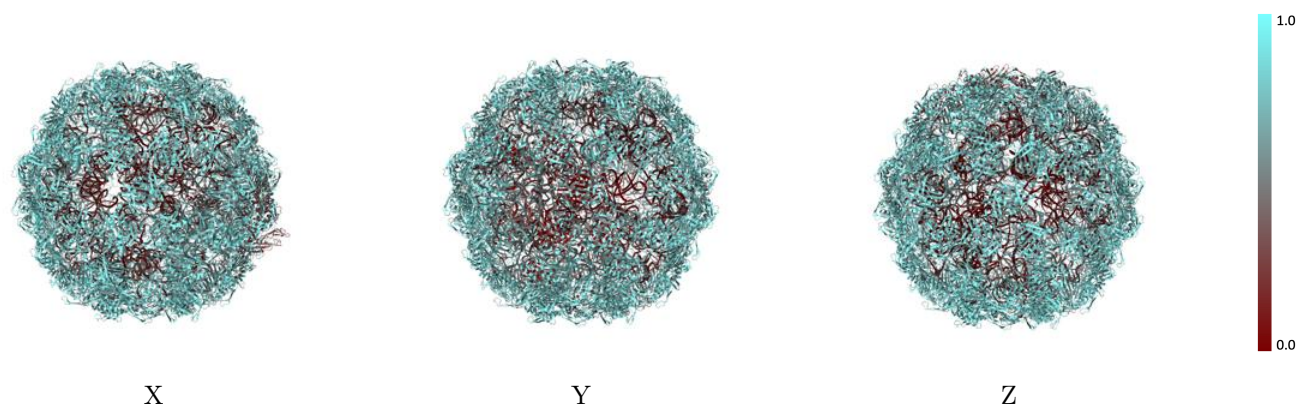
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



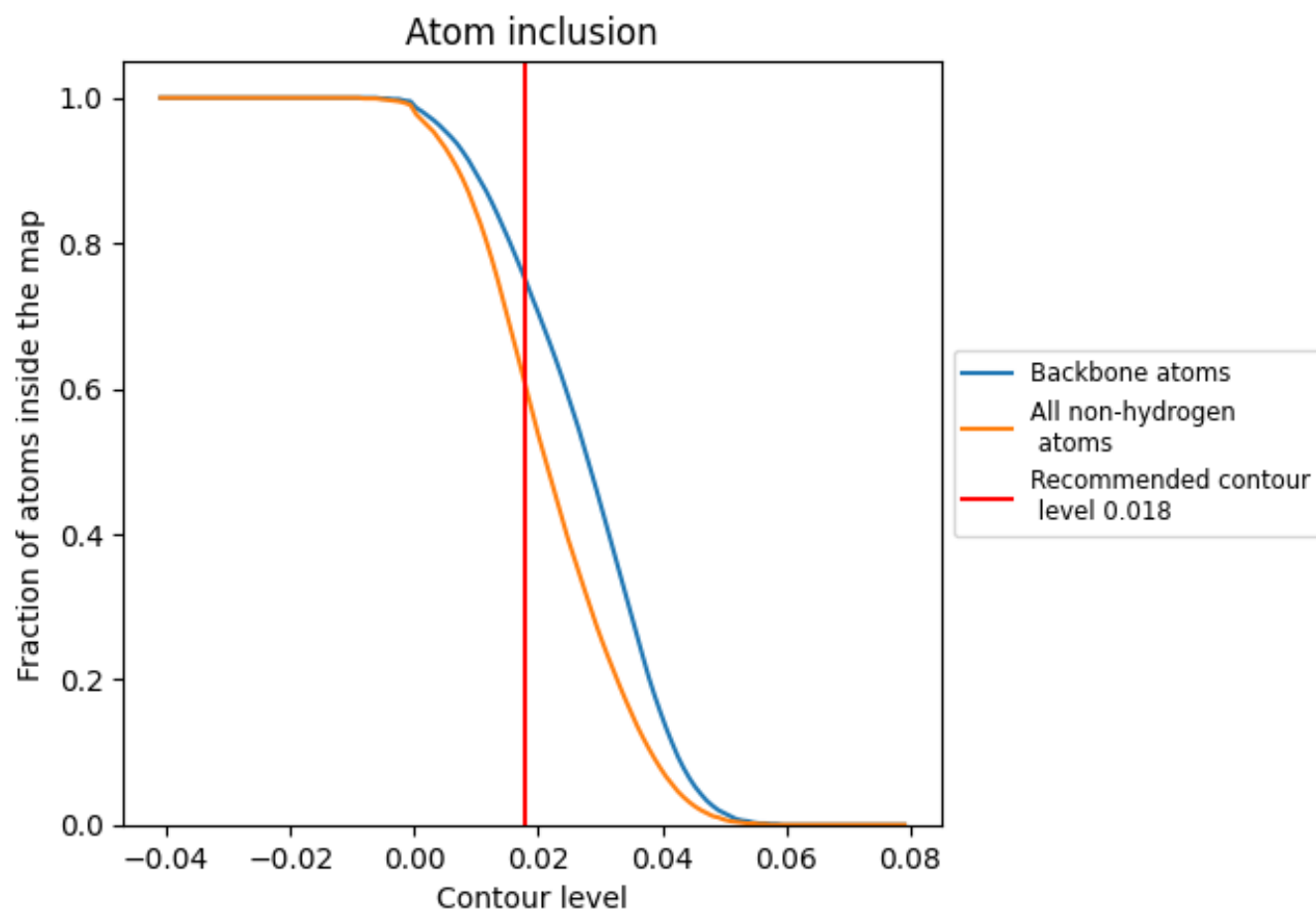
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6020	 0.2620
A	 0.3700	 0.1470
B	 0.1130	 0.0760
BA	 0.7340	 0.3420
BB	 0.7450	 0.3450
BC	 0.7550	 0.3500
BD	 0.7490	 0.3420
BE	 0.7710	 0.3540
BF	 0.7710	 0.3570
BG	 0.7660	 0.3570
BH	 0.7740	 0.3600
BI	 0.7240	 0.3490
BJ	 0.7570	 0.3310
BK	 0.7850	 0.3550
BL	 0.7420	 0.3510
BM	 0.7700	 0.3560
BN	 0.7810	 0.3680
CA	 0.7390	 0.3440
CB	 0.7670	 0.3370
CC	 0.7590	 0.3560
CD	 0.7620	 0.3600
CE	 0.7440	 0.3340
CF	 0.7650	 0.3520
CG	 0.7600	 0.3590
CH	 0.7740	 0.3490
CI	 0.8050	 0.3700
CJ	 0.7670	 0.3440
CK	 0.7590	 0.3430
CL	 0.7830	 0.3660
CM	 0.7320	 0.3440
CN	 0.7530	 0.3430
D	 0.1120	 0.0970
DA	 0.7520	 0.3480
DB	 0.7440	 0.3440
DC	 0.7490	 0.3360



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Chain	Atom inclusion	Q-score
DD	 0.7680	 0.3510
DE	 0.7400	 0.3280
DF	 0.7470	 0.3340
DG	 0.7600	 0.3560
DH	 0.7430	 0.3460
DI	 0.7630	 0.3480
DJ	 0.7840	 0.3420
DK	 0.7410	 0.3460
DL	 0.7550	 0.3310
DM	 0.7470	 0.3260
DN	 0.7100	 0.3230
EA	 0.7310	 0.3150
EB	 0.7720	 0.3330
EC	 0.7070	 0.3090
ED	 0.7020	 0.2550
EE	 0.6730	 0.2250
EF	 0.7090	 0.2960
EG	 0.5120	 0.1790
EH	 0.7200	 0.2670
EI	 0.7270	 0.3150
EJ	 0.7370	 0.3390
EK	 0.7400	 0.3390
EL	 0.7400	 0.3410
EM	 0.7230	 0.3020
EN	 0.7470	 0.3270
FA	 0.7210	 0.3140
FB	 0.5690	 0.1640
FC	 0.4310	 0.0920
FD	 0.4170	 0.1180
FE	 0.7030	 0.2800
FF	 0.5590	 0.1920
FG	 0.4910	 0.1460
FH	 0.6890	 0.2670
FI	 0.6710	 0.2610
FJ	 0.7540	 0.3320
FK	 0.7430	 0.3040
FL	 0.7250	 0.3090
FM	 0.7300	 0.3230
FN	 0.7600	 0.3400
GA	 0.7020	 0.2980
GB	 0.3250	 0.0850
GC	 0.5530	 0.1590

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Chain	Atom inclusion	Q-score
GD	 0.6890	 0.2740
GE	 0.7350	 0.3300
GF	 0.7300	 0.3280
GG	 0.7560	 0.3300
GH	 0.7750	 0.3510
GI	 0.7460	 0.3440
GJ	 0.7570	 0.3360
GK	 0.7650	 0.3510
GL	 0.7420	 0.3450
GM	 0.7580	 0.3510
GN	 0.7810	 0.3530
HA	 0.7350	 0.3470
HB	 0.7130	 0.3190
HC	 0.7630	 0.3510
HD	 0.7280	 0.3190
HE	 0.7440	 0.3160
HF	 0.7550	 0.3430
HG	 0.7370	 0.3270
HH	 0.7640	 0.3440
HI	 0.7890	 0.3660
HJ	 0.7700	 0.3520
HK	 0.7560	 0.3490
HL	 0.7560	 0.3640
HM	 0.7680	 0.3660
HN	 0.7620	 0.3420
IA	 0.7860	 0.3720
IB	 0.7730	 0.3590
IC	 0.7630	 0.3540
ID	 0.7870	 0.3650
IE	 0.7590	 0.3570
IF	 0.7430	 0.3530
IG	 0.7760	 0.3670
IH	 0.7510	 0.3370
II	 0.7660	 0.3340
IJ	 0.7900	 0.3560
IK	 0.7640	 0.3440
IL	 0.7740	 0.3490
IM	 0.7770	 0.3720
IN	 0.7450	 0.3550
JA	 0.7580	 0.3350
JB	 0.7620	 0.3450
JC	 0.7420	 0.3470

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Chain	Atom inclusion	Q-score
JD	 0.7500	 0.3440
JE	 0.7630	 0.3490
JF	 0.7370	 0.3380
JG	 0.7590	 0.3450
JH	 0.7530	 0.3390
JI	 0.7320	 0.3430
JJ	 0.7580	 0.3500
JK	 0.7830	 0.3600
JL	 0.7690	 0.3490
JM	 0.7610	 0.3490
JN	 0.7970	 0.3720
KA	 0.7440	 0.3510
KB	 0.7390	 0.3380
KC	 0.7560	 0.3390
KD	 0.7100	 0.3270
KE	 0.6040	 0.2110
KF	 0.7270	 0.2890
KG	 0.5710	 0.1930
KH	 0.7120	 0.3190
KI	 0.7320	 0.3110
KJ	 0.7220	 0.3270
KK	 0.7400	 0.3000
KL	 0.7530	 0.3400
KM	 0.7260	 0.3380
KN	 0.7610	 0.3540
LA	 0.7610	 0.3600
LB	 0.7460	 0.3410
LC	 0.7570	 0.3340
LD	 0.7590	 0.3510
LE	 0.7360	 0.3230
LF	 0.4680	 0.1430
LG	 0.6730	 0.2680
LH	 0.4190	 0.1080
LI	 0.6810	 0.2400
LJ	 0.5820	 0.1930
LK	 0.6690	 0.2710
LL	 0.7360	 0.3190
LM	 0.7510	 0.3360
LN	 0.7200	 0.2920
M	 0.4280	 0.2330
MA	 0.7560	 0.3340
MB	 0.7610	 0.3310

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Chain	Atom inclusion	Q-score
MC	 0.7280	 0.3280
MD	 0.7370	 0.3370
ME	 0.7580	 0.3600
MF	 0.7050	 0.3290
MG	 0.6910	 0.2760
MH	 0.7330	 0.3230
MI	 0.6990	 0.2980
MJ	 0.7580	 0.3150
MK	 0.7510	 0.3340
ML	 0.7420	 0.3370
MM	 0.7760	 0.3340
MN	 0.7550	 0.3440
NA	 0.7610	 0.3570
NB	 0.7500	 0.3520
NC	 0.7780	 0.3620
ND	 0.7350	 0.3370
NE	 0.7840	 0.3550
NF	 0.7700	 0.3590
NG	 0.7560	 0.3290
NH	 0.7450	 0.3390
NI	 0.7540	 0.3510
NJ	 0.7450	 0.3390